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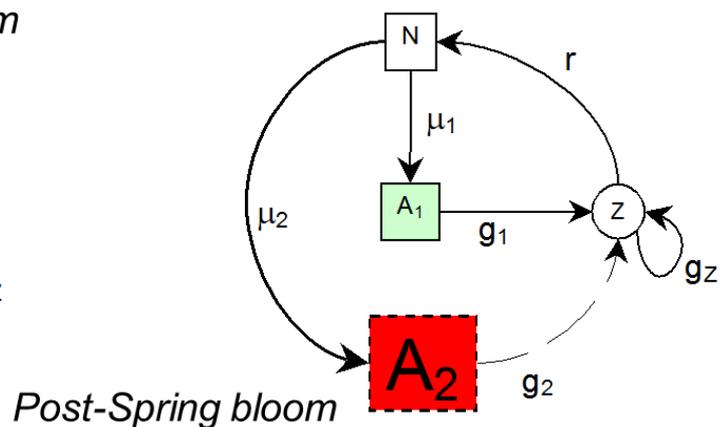
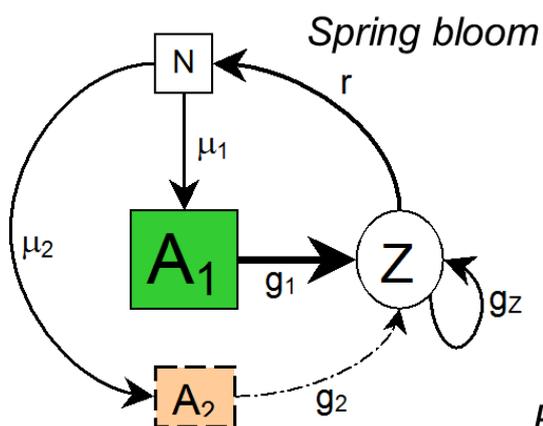
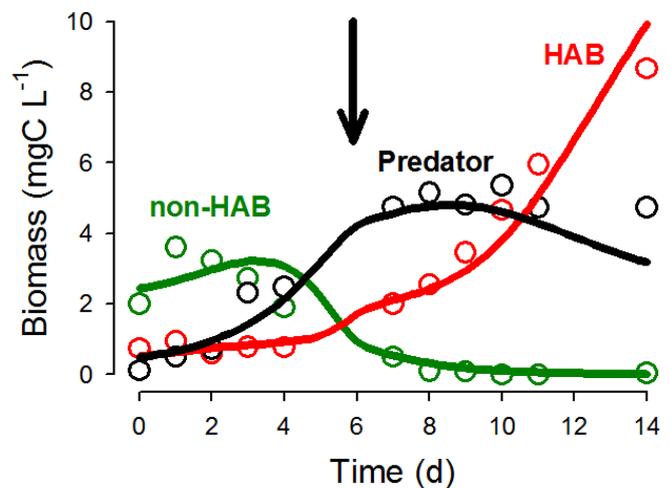
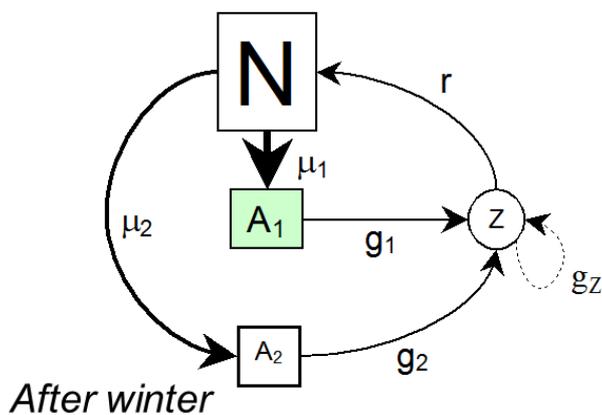
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Dynamic Ecology

an introduction to the art of
simulating trophic dynamics

Kevin J Flynn



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To my wife, Aditee Mitra, and our
son, Rohan Mitra-Flynn

In memory of:

Ian Butler (marine chemist and my PhD examiner): Ian worked at the Marine Biology Association (MBA) at Plymouth. Proud that he did not have a PhD (“it’s Mr Butler!”), he argued for the importance of dissolved organic nutrients in marine ecology at a time when the paradigm was against such nonsense. “We can’t all be perfect, can we, Kevin?!” said with a smile in his eyes whenever he was chastised over some triviality (never by me, I hasten to add). Given the importance now placed on DOM and the microbial carbon pump, I am sure he is smiling now.

David Cushing FRS (fisheries biologist): David was the founding editor of the *Journal of Plankton Research* (JPR) a journal that first appealed to me in my undergraduate days. I also found his text book *Population Production and Regulation in the Sea* an inspiration. Later, in the early 2000’s, and with Aditee Mitra, I helped to rebuild JPR, becoming its Editor for a while.

Mike Fasham FRS (oceanographer): It was Mike who, during the execution of a joint research project, decided that it would be better if I did the modelling of algal biochemistry and he “*just checked the code*”. This then forced my entry into this *in silico* world of ecological modelling. In between discussing plankton models, we talked about Merlin vs Griffon powered Spitfires, and other such distractions, over the odd pint of beer.

Paul Harrison, Eystein Paasche and Ted Smayda: Each an inspiring algal physiologist, and all suitably self-deprecating, perhaps never really realizing what excellent scientists they were and how important were their contributions to science. Importantly in the context of this book, they conducted the types of study from whence useful dynamic data series could be extracted.

Phil Syrett (algal physiologist): Phil was a superb scientist, BSc lecturer, BSc dissertation supervisor, and then my PhD supervisor. Never one for much talking, except on the subject of cricket (which leaves me cold), he was as sharp as a razor. His wife once said that, intellectually, I reminded her of Phil in his younger days; I could not ask for a better compliment, though I fear she was exaggerating somewhat as he was a far better scientist.

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Preface

This book aims to provide the biologist, and indeed the non-biologist (mathematician), with an introduction to dynamic ecology. The construction and operation of simulation platforms (models) provides an excellent test of understanding while also generating insight into how real complex processes in ecology operate over time.

There are various books available that are aimed at teaching biologists and ecologists how to model (e.g., Haefner 1996; Soetaert & Herman 2009; Jopp et al. 2011). Most, however, assume the reader is ofay with higher levels of mathematics and/or of computer coding than are most biology students. The language used within modelling (even excluding “statistical models”), coupled with the language used within different sectors of biology and ecology, also do little to help the novice. This text is intended to provide a platform for even the least maths-orientated biologist to engage with dynamic simulations. The emphasis is on building models with at least a nod to mechanistic (trait-based) functionality.

To provide a context for the models it is necessary to choose an environmental system. If I had gone for terrestrial examples (plants and insects, or especially enigmatic mega fauna such as wildebeests and lions) few would perhaps question my choice. I have actually gone for plankton. No, don't switch off - keep reading, please!

There are more plankton (numerically and by biomass), and they do more important things from a planetary perspective, than all the terrestrial animals put together. Plankton drive the ecology of the oceans that form the largest continual ecosystem on Earth. They have been crucial to the evolution of the atmosphere that supports most of the planetary ecosystems that we see today (namely through contributing to removal of CO₂ to limestone, and the release of O₂). Planktonic primary production generates ca. 50% of the oxygen we breathe. Plankton (as microalgae and as zooplankton, the latter such as water fleas) have also been widely used as exemplars of ecological systems in both empirical and theoretical research for very many decades. Even if you do not care about plankton, for much of what is here you could reword the examples with your favourite organisms, though for sure the spatial context of the system needs careful consideration. In consequence, the book will likely be of use to anyone with an interest in simulating ecological processes.

The book provides a step-by-step introduction to systems dynamic modelling, leading the reader progressively through levels of increasing complexity. Throughout, it is stressed that there are many caveats in the construction and deployment of all models, that while there is no single ideal approach there is also much scope for getting things wrong.

Chapters provide model descriptions through text and also through equations presented in a form to aid ready implementation in different modelling software platforms. Example outputs are given, so the reader can check that their own creations are operating correctly before they start to modify and otherwise develop their own models. Ideas for further exploration are also provided.

The work is supported by an Excel file containing all the model equations; this provides a ready route to deploy models in the readers preferred modelling software platform by copy-pasting equations. Complete, ready-to-run, models are also available for deployment within the Powersim Studio platform.

For further information, and updated models, please check www.mixotroph.org/models.

The Author

The author has written over 160 works (papers, book chapters) on various facets of plankton physiology, about half of which describe or utilise models. A particular emphasis in the authors' work has been on ensuring that models do not contain overly simplified, potentially dysfunctional terms. Across the breadth of plankton physiology the author has either conducted his own research on real organisms, or has worked closely with colleagues who have. This book brings together the basic concepts from two decades of developments in dynamic models, and experience in teaching the subject to undergraduate and postgraduate (research) students. The author published some commercially successful games for the Sinclair Spectrum home computer in the mid 1980's; those were written in hexadecimal machine code – no graphic-user-interfaces back then!

Further information on the research output of the author can be found at the following site:

https://www.researchgate.net/profile/Kevin_Flynn4

Thanks to

First and foremost I am indebted to the late Mike Fasham FRS (oceanographer), without whose enthusiastic support in the mid 1990's none of this would have come to pass. I also thank John Raven FRS (plant and algal physiologist) for inspiration. Thanks also to all those who have worked as co-authors on the shared papers that formed the bedrock of the approach taken in this book. I thank David Montagnes, Nathalie Gypens, Luca Polimene and Andrey Morozov for their comments on the penultimate version of this book. The final form of the book was also influenced by valuable inputs from several anonymous commentators, and by Ian Sherman at Oxford University Press.

The research that enabled this work was largely funded through various projects from the Natural Environment Research Council (UK) and the Leverhulme Trust.

Feedback Comments

Inevitably there will be mistakes (sorry!) and text can always be improved. I welcome any feedback that will enhance the contents of future editions. Please check at www.mixotroph.org/models for any corrections to model code.

Please email kjfplankton@gmail.com with any suggestions and comments.

Thank you.

Kevin J Flynn, May 2018

PLEASE READ ME FIRST!

The primary aim of this book is to help you better understand how ecology works, and critically how the dynamics function.

Much of ecology operates slowly, and often very slowly; that is so even when operating on a microbial scale such as within the plankton considered as exemplars in this book. However, through the use of simulations you can learn things very quickly, and you can experiment without fear of killing the system, or indeed without having to fill out ethics and health & safety forms.

Joking apart though, it is easy to become totally immersed in modelling and not take the breaks that you need for your own health. You are strongly advised to take a break every hour or so; go and walk outside and observe real ecology at work – it will stimulate your mind as well.

You can use this book in three ways:

1. You can work your way through it all, train yourself in some different approaches to systems dynamics, build and develop models upon your chosen software platform, run simulations and explore the numerous suggestions given at the end of most of the chapters. In general, equations in this book are given in a linear form similar in syntax to those entered into spreadsheets or most modelling and coding platforms. Equations can thus largely be copy-pasted from this e-book into your chosen modelling platform (noting that some level of editing may be required to conform with formatting needs; if you use Powersim Studio, it should all work directly). An MS Excel file containing all the equations in a form that is more immediately usable is available from www.mixotroph.org/models.
2. You could (largely) ignore the information justifying details of the construction that may otherwise train you to build your own models, and just transcribe the equations provided into your chosen software platform, run simulations and explore the suggestions.
3. You could just take the models made available via www.mixotroph.org/models, open them in Powersim Studio, and go and play. The smaller models will run in a free-download. For larger models you will need to purchase a licence. Go to <http://powersim.com/> to explore options; you may wish to check www.mixotroph.org/models for any further commentary on using Powersim Studio before purchasing a licence. You can then play with the simulations as you wish, and indeed develop and otherwise adapt the models. In time, likely (indeed, hopefully) you will re-read the book and go to option #1, above.

For more on software options, see Chapter 2, Section 2.7.

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1. Introduction

Terms and concepts introduced in this chapter- plankton types, functional types, stoichiometry, models vs simulations, statistical vs system dynamics models

1.1 What Is In This Book

This book contains an introductory guide to get you started in modelling dynamic ecology, covering the interrelationship between conceptual and empirical models, and deterministic systems dynamic models. The book does not cover matrix, statistical, stochastic or other such approaches.

In essence, the book aims to provide an introduction to the modelling of ecology as it relates to the flows of material between biological and abiotic components of the ecosystem over time. Of course statistical models (as regression line fits) may be driven through data within time series. The presence of time as the x-axis on a plot reporting “model output vs data” is thus not indicative that a simulation model has been used. Many biologists and ecologists are caught by this confusion. It is safest to explicitly refer to models as *statistical*, *dynamic* or *simulation* to differentiate between these approaches.

To provide a point of reference, the book is based upon plankton ecology; for justifications, see Section 1.3. The book works through from very simple (often technically highly questionable) descriptions of biology and physiology through to more complex creations. These biological entities are operated within a simple framework describing the physical and chemical environment. The abiotic components are also described in simple terms, but with sufficient complexity and variety to demonstrate that the environment can easily have an overwhelming influence on the dynamics of ecology. By the time you have worked your way to the end of this book you will be well equipped to either develop and run your own physiologically detailed creations within simple abiotic frameworks, or you will have also expanded the physical description (perhaps to planetary scales).

1.2 What, Why – Dynamic Ecology

Ecology is the study of how organisms live together in their environment. The interactions between those organisms, how those interactions are tempered by the abiotic features, and indeed how over short and long terms the abiotic environment is affected by life, are all dynamic. It is not possible to study ecology fully without understanding the underlying dynamics, and yet most students of ecology have little appreciation of what those dynamics truly represent and how they interact at different levels and with different rates.

Most effort in ecology is expended on monitoring subsets of activity with little attempt to literally balance the books with respect to energy and matter. Consider that rabbits eat grass and are in turn eaten by foxes. At a very basic level these interactions involve the transfer of material between organisms, and yet how many ecologists actually measure those transfer rates and relate them to resource supply and demand? The dynamics of such interactions, which are typically cyclical, are representative of what are termed complex adaptive systems that drive what we see

happening in our world. And humans are an integrated part of that world. In agriculture, aquaculture, sewage treatment, anaerobic digestion etc., humans manipulate ecology; the study of dynamic ecology is just as important in an applied setting as in a natural, wild, one.

Modelling and simulating dynamics provides a very powerful way to explore, develop, test and exploit understanding. This applies as much to ecology as it does to manufacturing and finance. The skill sets are highly transferable. Applying those skills also makes you think in a different way, helping you to conduct empirical research in ways that provide information that can be more readily exploited to build models which then, in turn, enhances understanding through studying the simulations. Modelling should not come after studies of ecology (or indeed studies of any dynamic system); they should be immersed within the whole effort. This work is targeted not at modellers and mathematicians, but at biologists and ecologists. Arguably an ability for biologists and ecologists to build and exploit dynamic models should be as common as their use of statistics. If you cannot model and simulate the system you study then you do not likely have sufficient information to even attempt to fully understand it.

1.3 What, Why – Plankton

The largest continuous ecosystem on what should arguably be called planet *Ocean*, is marine. The ecology of this system is driven mainly by planktonic activity; that is by a food web comprised of organisms that effectively drift in the oceans. Plankton inhabit primarily the upper sunlit zone of the oceans, a zone which is very shallow (often only a few 10s of metres deep) in comparison with the average depth of the oceans, which is over 3.5km. Lakes and ponds also contain planktonic organisms; these may be of local importance perhaps as nuisance organisms contaminating drinking reservoirs, or for support of aquaculture or biotechnology.

Plankton can be divided into groups according to size and functionality. *Viral-plankton* and *bacterio-plankton* are (obviously enough) viruses and bacteria, respectively. In contrast, *phytoplankton*, which are traditionally considered as “microscopic planktonic plants” driving primary production, include the prokaryotic cyanobacteria (“blue-green algae”) as well as the eukaryotic phototrophic protists. Neither of these types should ever be technically considered as “plants” in any shape or form. Much of the secondary production in this ecosystem is performed by the *microzooplankton*; these are protists that eat, typically through a process called phagocytosis. Recently we have (belatedly) come to appreciate that most of the protist “phytoplankton”, and a good proportion of the “microzooplankton” are actually mixotrophic; they are single celled organisms that photosynthesise and eat (Flynn et al. 2013; Mitra et al. 2016). For simplicity, and in line with an introduction to dynamic ecology, in this book we will restrict ourselves to the traditional, if flawed, dichotomy of phytoplankton and zooplankton. While these protist plankton are almost all sub-millimetre in size, the metazoan zooplankton (classically including copepods and freshwater water-fleas, but also including the larval stages of many benthic organisms, such as barnacles, sea-stars, crabs, and also larval fish), range in size from smaller than the largest microzooplankton to larger than many fish (namely, sea jellies).

Size-related naming conventions divide plankton according, at the lower size groups, to their fresh weight, as per Table 1.1. Although few plankton are spherical in shape, by convenience their size is often given as an “Equivalent Spherical Diameter” (ESD). The prefix “micro” may, confusingly, refer to any/all plankton that are so small that a microscope is needed to observe them (typically < 1mm), or to a specific size range (20-200 μm), or to microbial plankton (i.e. prokaryote or single

celled protist, which could be anything up to 1mm). The size range for even the microbial plankton is in relative terms massive, ranging from $<1\mu\text{m}$ bacteria to 1mm microzooplankton; that is a biomass range equivalent to mouse -to- cow.

| Name | Fresh weight | Equivalent Spherical Diameter range (μm) |
|----------------|---------------|---|
| pico-plankton | pg | 0.2 – 2 |
| nano-plankton | ng | 2 – 20 |
| micro-plankton | μg | 20 – 200 |
| meso-plankton | mg-g | 200 – 20000 |

Table 1.1 Size-descriptors for plankton. Above these are the “macro-plankton” (2-20cm) and “mega-plankton” ($>20\text{cm}$).

Planktonic organisms are not necessarily immobile. Many can move at rates not dissimilar to the swimming speed of fish when considered in terms of body-lengths per second. Some microscopic plankton undertake daily vertical migrations of many metres, or even 10s metres – quite some undertaking for organisms that are mere fractions of a millimetre to a few millimetres in length.

And these organisms can certainly be photogenic! Figure 1.1 gives just a very few examples. See also <http://planktonchronicles.org/en/the-project/>.



Fig. 1.1 A few example plankton. Photo credit John Dolan, CNRS.

While plankton are typically microscopic, their collective activity has over hundreds of millions of years changed the face of Earth, contributing significantly to the formation of limestone rocks, to the deposition of gas and oil, and especially to the formation of an O_2 -rich atmosphere; currently, marine planktonic primary production contributes ca. 50% of the O_2 we breath.

Planktonic activity not only continues to affect the functioning of the planet in the broadest sense, but they support the food web that ends with fish and megafauna (most obviously the plankton-

eating baleen whales). In very large measure the existence and ecology of the enigmatic megafauna that so captures the attention of the public (as fish, sharks, squid, whales, turtles, seabirds etc.) is shaped by the planktonic activity about which the public know little or nothing. Only when something goes wrong, such as a harmful algal bloom (HAB) causes a fish kill or a beach becomes covered in stinging or rotting sea jellies, may plankton enter the public consciousness.

Without any doubt, then, plankton ecology needs little justification as an important subject in its own right. However, the apparent simplicity of the plankton food web (in terms of the traditional phytoplankton-zooplankton dichotomy; see the cover illustration and Fig. 1.2) and the apparent homogeneity of the physical environment also presents theoretical ecologists with an ideal platform for explorations of how organism-organism interactions may play out in a generic sense. *Apparent simplicity*, because now we recognise that most sunlight-zone planktonic protists are actually mixotrophic (undertaking both primary and secondary production in the same cell), we can also see that things are somewhat more complex than scientists have typically considered. In addition, the so-called homogeneous environment is only really viewed like that in reflection of a human-centric concept of space and time. Almost the first thing an aquatic ecologist will do when provided with a water sample is to shake it to ensure the contents are indeed mixed homogeneously! In reality, plankton clump and swim towards or away from physico-chemical clues (most obviously light, but also chemical scent trails from chemicals leaking from organisms) forming local patches of higher organism abundances.

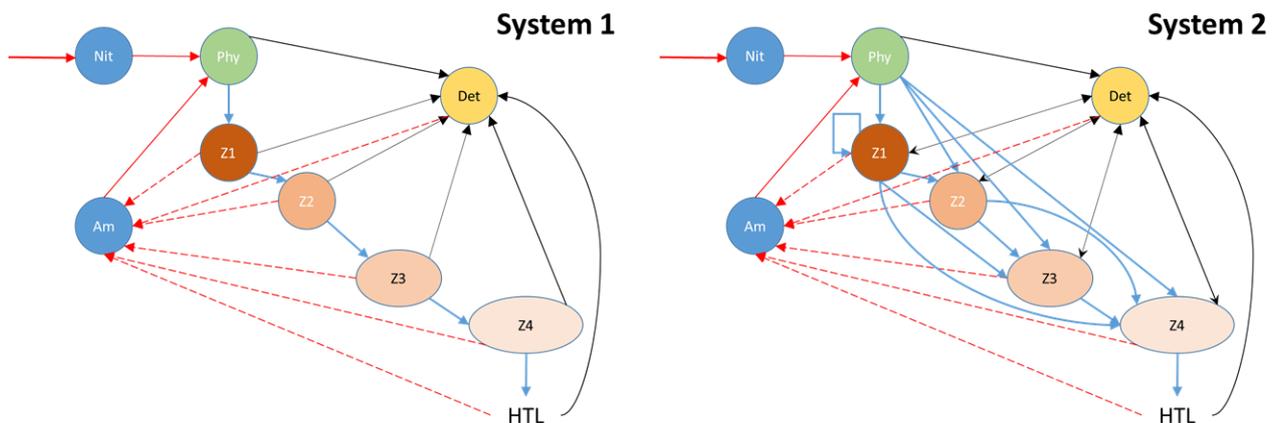


Fig. 1.2 Example conceptual planktonic food webs. System 1 shows a simple linear food chain from phytoplankton (Phy) through a chain of zooplankton (Z1-Z4) and higher trophic levels (HTL). The nutrient is nitrogen, which enters the system as nitrate (Nit) and is regenerated as ammonium (Am; red dashed connectors). All organisms contribute to detritus (Det; thin black connectors) with its allied bacterial community. In System 2, the simple food chain is replaced with a complex food web, including a cannibalism link for Z1, and use of detritus by the zooplanktonic consumers. The complexity of such trophic constructs in nature varies greatly, and likewise you can make your simulated description as simple or as complex as you wish. By the time you have reached the end of this book you should be able to build something akin to System 2 and operate it under different abiotic conditions.

The short life cycle of most plankton, with many organisms having doubling times in the region of hours to a few days, and that many millions of individuals may occupy a single litre of water, facilitates the undertaking of experimental studies in support of theoretical concepts. Couple this

with the relative (or apparent) ease of categorising plankton into different **functional types** (that is, into groups of organisms that fulfil specific “roles” in ecosystem function) and it is easy to understand why plankton are such popular experimental subjects. The size range also facilitates explorations of allometric (size-based) relationships, while the **variable stoichiometry** (most obviously with respect to organismal elemental C:N:P) within and between planktonic organisms aids studies of what has become an important driver in current thinking of dynamic ecology, namely **ecological stoichiometry** (Sterner & Elser 2002).

In short, plankton ecology is a highly significant process on Earth, and it also presents an important, valuable, generic ecological structure for study.

1.4 What, Why – Model vs Simulations

What is a model? In crude terms, a model is a simplification of reality. Models come in different forms; for example, they may be physical (model aircraft, or indeed physical models of planktonic organisms), conceptual (schematic or pictorial, such as illustrations of food webs or of biochemical pathways), or mathematical. Mathematical models themselves range from simple linear regression fits through data sets (so-called “statistical models”), through to descriptions of fluid dynamics with particle tracking over time.

We also need to make a distinction between models and simulations. A model as a simplification of reality could be so simple, or so abstract, that it does not well represent reality at all. Thus, there are model aircraft that do not resemble in any way real full size aircraft, except that they fly after a fashion. Many models of aircraft do not fly either, being static items for display only. The term “simulation”, and thence simulator, is more suggestive of a reproduction of a real event or system. A critical feature of a “simulation” is that it is time-based, and a major use of simulators is to project future developments. In consequence, while there are many different types of ways to model plankton, only a subset of those may be used with some justification or confidence in simulations.

At the end of the day, what is important is that the developer, user, and interpreter of the model output appreciates (with reference to the simulated system) the rationale under which the model has been constructed, the ways in which simplifications have been enacted, and thence the implications for how well the output may simulate reality. The ability of a simulation to match current-day reality may then be indicative of how robust the model output may be when run in a “what-if” scenario, operating under conditions beyond those used for model testing. Recall that this type of operation, predicting beyond the bounds of extant knowledge, is deeply frowned upon when extrapolating beyond the data used for the construction of a regression line. Only if we have very strong mechanistic underpinnings for such regression lines should extrapolation be undertaken; the same caveat applies for models used for simulating the future world.

And this brings us to “why model”. To build a model that can indeed simulate reality to a level of agreed confidence is an excellent test of what we know about an ecological system. If we understand the system, then we may be able to simulate its behaviour under different conditions; if we cannot model and simulate with confidence, then we do not understand the system sufficiently. For applications in biology, here on plankton, this helps to set the division between natural history and natural science. Interestingly, some of the most heated discussions that can occur during model development or at scientific meeting are not about model construction itself,

but concern disagreements over the relative importance of this or that facet of physiology. Ironically, a well-constructed model can help to resolve that very conundrum; but that is rather a chicken-and-egg problem.

There is often repeated a claim (attributed to the statistician Sir George Box FRS) that *all models are wrong, but some are useful*. I will argue in Chapter 7 that you should never use a simulation model that is wrong (= unsuitable, incorrect). A model is inevitably going to be incomplete, and you have to decide where gaps will be tolerated; that is certainly where *some are useful* may be applied. But that is not the same as being *wrong*. Another point is that Box was referring to statistical models which are very different in their scope and applicability in comparison to systems dynamic models, as considered here. Of course, you have no control over what someone else may do with your model, and they may indeed use it in a situation for which it is ill configured (*wrong*, if you like). You, as a builder of models, have the responsibility to build a model that is robust (not likely to accidentally go *wrong*) and to adequately document it. The onus is on the user to verify that the model construct is (still) fit for purpose and establish its limitations when operated in a different situation.

2. Modelling Tools & Approaches

Terms and concepts introduced in this chapter- model types, system dynamics, systems biology, systems biology, naming variables, variable types, integration, units, deterministic vs stochastic, functional types, biomass vs individual based models, system balance conceptual/structural and mathematics checks, sensitivity tests

The purpose of this chapter is to introduce some terms and concepts. These will be explored further in later chapters, but it is likely that you will need to return to this chapter for definitions and guidance. It is recommended that you read this Chapter, and also Chapter 3, in their entirety before continuing to the modelling chapters themselves.

2.1 Introduction to System Dynamics Models

The models described in this work fit into a branch of mathematical models that may be termed Systems Dynamic Models (**SDM**). Such models describe changes in a system over time, usually exploiting differential calculus. Specifically, these models use ordinary differential equations (**ODEs**). It is important to appreciate that you do not need to be overly mathematically literate to make use of SDM approaches. Indeed, you do not need to have mathematical skills above those of a typical 16yr old; please read Section 2.6 if you have concerns on this matter. What is far more important in the context of this book is that you think in terms of how biology, from biochemistry to ecology, actually functions.

SDMs are often produced specifically to simulate real processes; thus SDMs are used in business and finance, to describe stocks and flows through manufacturing and commercial activities. SDM applications in ecology could include describing events such as the transfer of nutrients from the soil into plants, from the plants through a chain of animals and microbes and back to nutrients in the soil. Here we consider the use of SDMs as tools to explore the dynamics of ecology as represented by planktonic interactions (see Chapter 1 for an explanation and justification). SDMs may thus find a role in biochemistry (where the science may be termed **systems biology**) through to ecology (termed **systems ecology**).

The process of model development and use, and how this interacts with non-modelling approaches is illustrated in Fig. 2.1. The important take-home message is that modelling should not be viewed as an endpoint in research, as something to do when all the empirical research has been conducted. Thus, while it may be tempting to consider the processes involved in building simulation models as linear (concept, build, test, deploy), in reality the process is cyclic with empirical data and the conceptual framework being reconsidered in the light of explorations of model behaviour and, in due course, as our understanding of the system develops.

The cyclic process in building and using, or exploiting, dynamic models is mirrored in the structure of this book. The ways in which even the most simple model can be built into a complex form inevitably means that choices have to be made as to when to introduce which modelling concept or approach. Each major modelling chapter in this book represents an increase in conceptual and/or modelling complexity, starting with a section explaining why and how we got to this stage, and ends with a section considering how to develop the model further. You will in consequence

likely read and then re-read some sections in a new light as your understanding and interests develops.

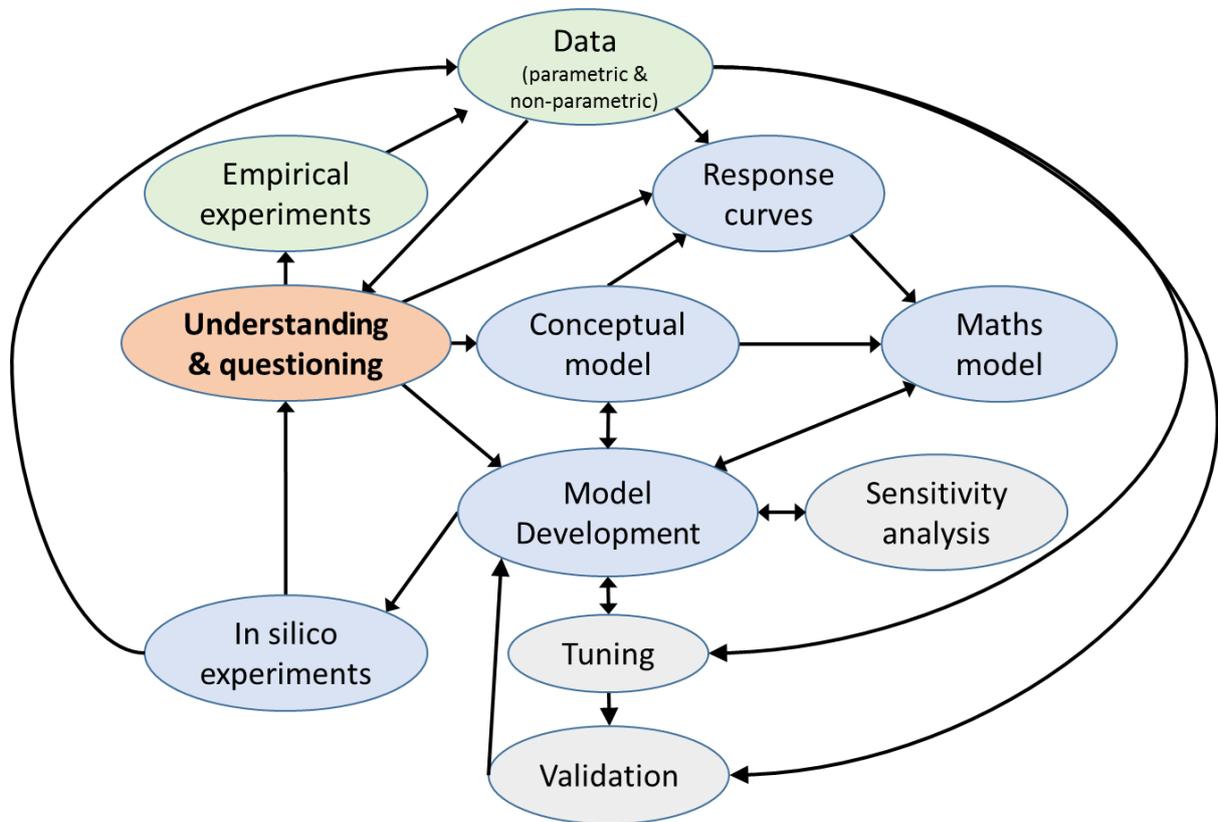


Fig. 2.1 Schematic showing development steps in dynamic model formulation and deployment, and how these interact with empirical ecology. Science progresses through iterations of how we understand the world and consequential questions (what-if? etc.). From those questions formal hypotheses and empirical experimentation develops leading to new data (initially as simple observational non-parametric studies, or “natural history”, and then increasingly parametric). From understanding we can also develop conceptual models (diagrams of biochemistry, food webs, biogeochemical cycle etc.) from whence mathematical models are developed through combinations of developing response curves (relating inputs to outputs etc.; see Section 4.3) and iterations of model development and testing (sensitivity analysis, tuning to data, validation; Chapters 13 & 14); see also Section 6.9. The mature model is then deployable as a platform for conducting in silico experiments contributing to understanding and generating new questions.

The book takes planktonic systems as its exemplar. Such systems can be very simple (just one or two species growing in a flask for a few days) through to extremely complex (dozens of different groups of organisms ranging over the oceans, simulating production cycles over decades). See Fig. 1.2 for an example. Even the simplest system could be modelled to a high level of complexity, considering biochemical feedback regulations of physiology within each of the organisms simulated. It is this challenge of simplicity versus complexity that at once provides inherent fascinations and frustrations to the modeller. In consequence the modelling process can never be considered as complete. In turn, this requires that the modeller maintains a rigorous level of documentation and quality control, justifying (if only to themselves) what they have done, why, and how.

2.2 Keeping Track of Progress – The Need for a Log

Anyone who uses spreadsheets of any size will know how easy it is to become “lost” in the detail when they have not looked at the file for a week or so. Working with models is much worse! It is for this reason that frequent updating of a log, and rigorous documentation within the model file itself, are essential. Saving new variants of the file (i.e., with a new version number or name) is also invaluable. Being methodical is especially important when you come to tracing and removing errors in the model, a process termed **debugging**. It is all too easy when debugging to make a series of changes that make matters worse and that need to be retraced and undone. The log could be pen-and-paper, but more usefully it would be as a text (word processor) file which can be easily searched by keyword.

2.3 Variable and Parameter Types

Mathematic models comprise equations that inter-relate variables. A variable is a characteristic, an entity or feature, which changes. A parameter is a characteristic that does not change. In models, almost every characteristic is technically a variable. The only characteristics that are strictly parameters would be physical constants such as acceleration due to gravity, or molecular mass.

SDM models contain 4 main variable types:

State variables (or “levels”):

These describe quantities that can typically be literally held or captured, such as biomass, nutrients, or organism numbers. These variables are, relatively speaking, easy to measure and it may be tempting for a biologist to wish to include many state variables in their models. In practice there are good computational reasons to keep the count down; computational effort is mainly attributed to calculating inputs and outputs to state variables, so the more state variables you use the slower the model will run. There are also good practical reasons to restrict the number of state variables, else the biologist needs to measure very many variables and that is typically a complex and expensive undertaking (and is often impracticable as well).

A classic challenge in ecology is simply measuring the biomass of different organisms. How do you measure the total biomass of a plant, including its roots? With plankton, typically it is not possible to separate sufficient quantities of each organism type for weighing or chemical analysis, so the best that can be done is to determine the total population biomass (usually by elemental analysis of the organisms collected from a few litres of water onto a filter), and to estimate the size and abundance of the different organisms by microscope, or similar. From the latter, assuming you have a size-based relationship to biomass for individuals, the population biomass can be estimated and allocated between groups. Such relationships with size are termed **allometric**; the relationship between size and C-biomass varies between taxonomic groups in plankton (Menden-Deuer & Lessard 2000).

Constants:

These describe characteristics that, at least within the time course of the simulation, are held invariable during the simulation. That is to say, they are viewed as parameters (hence the terminology to “parameterise a model”; Chapter 14).

Examples of characteristics that are technically variables which are typically held as constants include maximum growth rates, maximum or minimum organism size, and half saturation constants for biochemical processes. It is rare that “constants” are really of true fixed value; “constants” may be better thought of as input variables than as true parameters. Indeed, in many instances it may be desirable to drive so-called constants from an external database. An example would be to replace a fixed set of values for light, temperature and humidity with input variables to describe the local weather (we will use this approach in Chapter 10). A simple count of constants does not itself necessarily indicate how challenging a model may be to configure. It depends on what the constants describe. You can also bury constants as numbers within equations, which rather disguises the real number of constants in the model.

Auxiliaries:

These are intermediaries in calculations, being described by an equation that usually updates the numeric value at each time step over the duration of the simulation. There may be additional auxiliaries that are not strictly required to run the model, that provide transforms to give outputs in units more typical of the research arena of interest (such as μM computed from mg m^{-3}). The numeric value of an auxiliary may not actually vary during a simulation. It may de facto be a “constant”, representing within the model structure a transform, for example.

Sometimes the modeller may break up a long complex equation into several smaller steps, in order to clarify or simplify understanding, using several auxiliaries rather than one long complex equation. A count of total variables so as to compare model complexity can thus be misleading if it includes a count of auxiliaries.

Flows:

These describe the flow of quantities into and out of state variables. Because they describe rates, their units always include “time⁻¹”, or “1/time” – that is “per time”. Flows may be described by a constant, but more typically they vary during the simulation as functions of other factors, such as resource availability or population activity; flows are thus usually described by auxiliaries. Accurately measuring rates within real biological systems is typically very difficult, not least because the very process of measuring rates typically affects the rates being measured (e.g., for nutrient uptake into phytoplankton; Flynn 1998).

A common feature of ecology and biochemistry, and of dynamic systems in general, are **delays** in flows that alter the dynamics of the state variable values. Some of these events may appear rather obvious, such as the consequence of organisms having resting stages (hibernation, seeds etc.), or in matching between predator-prey cycles, while others are perhaps less obvious (delay in satiation controlling further predatory activity). In part, the importance of delays to the system you are studying depends on the duration and nature of the delay in the context of the broader system dynamics. If you are modelling events over a whole year, then a delay in predator activity in response to prey availability of a day or so will most likely be of no consequence. The same event considered over a two week prey growth cycle could be highly significant.

Some modelling platforms simplify the simulation of delays by running a routine akin to a conveyor belt; a number is input to the function and reappears at some selected time in the future. Such a function may be termed as “pipeline-delay-function”. More often than not in biology some loss of material or organisms will occur concurrently with the delay. Thus, not all seeds will germinate because a proportion will die or otherwise fail to germinate.

2.4 Documenting Information about Variables

Every variable should have the following items recorded against it.

Variable Type:

“State variable” (with the input and output flows), “constant” or “auxiliary”

Units:

The full units should be documented. For example, what are called “specific growth rates” formally have units of only time^{-1} . However, it is always best to document C-specific growth rates explicitly as $\text{gC gC}^{-1} \text{d}^{-1}$, chlorophyll-specific growth rates explicitly as $\text{gChl gChl}^{-1} \text{d}^{-1}$, etc.; this provides the reader with useful information on the source of the data.

There may be no units, in which case the unit is dimensionless; it is as well to document that condition (“dl”) to indicate the status, rather than perhaps giving the impression that the unit has been forgotten. If appropriate, it is also useful to include the full units that contribute to an apparent unit-less status (e.g., gC gC^{-1}).

Units must balance across equations; whatever you do with the numbers you do with units. Indeed, undertaking this unit calculation is a useful way to help check model structure. For example, you can only add together variables that share the very same unit (see Section 2.11). Some software packages attempt to check units; this can be most useful, but it can also be annoying in practise.

Array index:

A variable may be arrayed to further characterise it, using an alpha-numeric index given after its name. In simple models there is a single array, which does not need to be stated. In complex models there may be multiple array indices. For example, the state variable “*fish*” could carry indices describing species, and pond; thus *fish*(1,2) could refer to fish species 1 in pond 2. There are many uses of arrays, primarily associated with making the code more compact, but we shall not consider them further in this book.

Documentation:

Documentation should be sufficient for someone other than the author (or indeed the author!) to enable an understanding of the role and origins of the variable, and the functioning of equations.

2.5 More on Units

SI units for dimensions, volumes and time are m, L and s. While you could argue to use these units in your models, in practice this is not necessarily very useful or helpful.

Growth rates for plankton are most usefully described with a time unit of day; division times for phytoplankton are around 1 day, synchronised by the diel light-dark cycle. It is thus most likely that you will wish to use “d” as the time unit for your models. However, when considering motility, units more in keeping with the dimensions of the organism may seem more appropriate, thus swimming speeds with units of $\mu\text{m s}^{-1}$ may be used. Units of diffusion are often given in $\text{cm}^2 \text{s}^{-1}$.

For units of mass and concentration, you could use moles L^{-1} (do not use M, as that applies only to dissolved compounds, rather than to solids such as organisms). More often g L^{-1} or g m^{-3} are used. Or you could use $\mu\text{g L}^{-1}$, or mg m^{-3} ; these two alternates have the same numeric value, of course. So, $1\mu\text{M}$ nitrate-N would be $14 \mu\text{gN L}^{-1}$, or 14mgN m^{-3} . For models applied to field applications, working in m^3 feels appropriate, while for laboratory studies conducted in flasks, using L may be preferable. However, if you need to use linear and volumetric dimensions in your model then units of L may not seem very helpful, as the linear dimensions for L are $(0.1\text{m})^3$.

In practice then, different models and different modellers, use different units. This can cause problems when transferring equations between sub-models and applications unless you keep track of them (see Section 2.11 and Chapter 3). Throughout this book, no specific attempt has been made to harmonise units between all chapters, as applications differ.

2.6 The Background Mathematics; integration methods

Before reading on, if you have not studied higher mathematics, do not worry. A detailed understanding of the underlying mathematics is not required, especially if you are using specialist modelling software (see Section 2.7). **You may find it easier to return to this section later; you do not need to read this in detail now.**

Most SDMs use ordinary differential equations (ODEs) to calculate flows of material in and out of state variables. This process exploits **differential calculus**. Very crudely, the equations calculate the **rate of change** of the value of the state variable per unit time. You will likely have seen such rates of change described as “ dy/dx ”; in simple terms this can be read as “{difference in variable y }/{difference in variable x ”}. In the models described here x is time (t), so dy/dt is more appropriate.

Most students encounter differential calculus at school, at the level of differentiating an equation in order to determine rates of change. Later, they may encounter the opposite of differentiation, which is a form of calculus termed **integration**. Integration is the process actually used in SDMs; the user provides the initial state variable value, and equations that describe the rate of change, and the integration process calculates the value of the state variable at the next time point. And so on over the duration of the simulation. With simple systems of equations, integration may be achieved analytically; that is typically the case for school-level calculus. However, in complex systems this is not possible, and integration is achieved numerically, through a series of iterative calculations called numeric integration.

So what happens at each time point? If you know the value of the state variable (for example, the biomass) at two time points, then you can compute the rate of change over that period. That is what you measure during an experiment. However, if you know the initial biomass, and the rate of change, you can calculate the new biomass; this is what the modelling software does to simulate what is happening to the biomass as time passes.

In SDMs the value of the rates into and out of state variables (i.e., flows), are defined by ODEs linking the value of constants, auxiliaries and state variables. The process of integration within the software takes the value of that flow (which, recall, has units including 1/time), to compute the flow over a fraction of time. That fraction of time is termed the **integration time-step**. This time step sets the frequency with which the numeric integration routines operate. You may think that the more frequent (the smaller the time-step), the better. However, frequent calling of these routines slows the simulation so in reality a balance is struck between using a step size that is small enough to ensure the process of integration is adequate (mathematically accurate enough), but not much smaller. The most obvious symptom of the step size being too large (the calculations are not done frequently enough) is of the values for state variables escaping accepted bounds; for example, the state variables reporting biomass or nutrient values become negative. The more rapidly the dynamics of the simulation change, the smaller must be the time-step in order to resolve the dynamics satisfactorily and prevent errors creeping in.

There are several computational routines used to achieve numeric integration; most platforms support routines named *Euler* and *Runge-Kutta (R-K)*. The software platform that you use needs to support at least one form of integration. That may include different levels of the same integration, thus there may be R-K1, R-K2, R-K4, K-K4var. The number refers to the number of times at each time-step the routine operates in order to improve the accuracy of the solution. In a variable time-step routine, such as R-K4var, the time-step itself is also altered (varied – var) so that when little is changing in the simulation then the time-step is automatically made longer (cutting computational effort), and conversely made shorter when events are changing rapidly.

It is not necessary here to understand how these methods work, though there are important differences between Euler and R-K which are worth appreciating (check for debates on the topic in online forums). Especially at higher iterations of R-K (e.g., R-K4), the R-K approach is more accurate, though (as more calculations are undertaken at each time-step) inevitably it is slower.

For applications to SDM the judgement as to which method to use may readily be gauged by comparing outputs of the model using different methods, with respect also to the run time of the model. R-K4 may be considered the safest bet from a mathematical standpoint. There is one important point to note though; the Euler routine can be used to empty a state variable to zero, while typically that is not so with R-K. Interestingly, computer gaming programmers tend to use Euler type approaches as they are faster and more robust (the software is less likely to make a computational error and crash), even if ultimately the method is less accurate. SDM models tend to be robust as they account for materials flowing around system; see in contrast for example Chapter 6, legend to Fig. 6.4. **Unless otherwise indicated, all models described in this work were operated using the Euler method to generate the plots shown.** Running them with R-K4 makes little difference to the outputs in most instances, except the run time is longer. You should always check your model under different integration routines, as well as using different integration time-steps. Do not become overly concerned with minor differences; if there is a significant difference it will indeed be significant (i.e., obvious)!

2.7 Modelling Software

You need to run models using an appropriate software platform. Using an internet search engine for “dynamic systems model” will return various options for constructing and running models.

The platform used by the author is that provided by *Powersim Studio* (powersim.com), to operate in a Microsoft Windows environment. Various other options exist, such as *Simile* (simulistics.com; for Windows, Apple Mac, Linux), *Stella* (iseesystems.com; for Windows and Apple Mac), and web-based platforms such as *insightmaker.com*. At the other extreme, and for maximum speed, you could use FORTRAN, Python, C, or another coding language.

Bespoke modelling platforms typically use a graphic user interface (GUI), with the mathematics hidden from immediate view. Such interfaces use different symbols to denote variable types. The classic example for DSM is the **Forrester diagram**, after the computer engineer and systems analyst, Jay Wright Forrester. In such diagrams, boxes denote state variables, diamonds are constants, and circles are auxiliaries. An example is shown in Fig. 2.2. Flows between state variables are shown as pipes with arrows showing the direction of flow (a negative flow rate is thus backwards), and a “valve” symbol linked to either a constant (diamond) or more commonly to an auxiliary (circle). If there is a source or sink for material outside of the explicit concern of the model then this shown as a cloud symbol attached to the pipeline leading to or from the relevant state variable (e.g., Chapter 6, Fig. 6.1). Linking these symbols with arrows and pipes not only acts to illustrate linkages between variables in what many would consider an intuitive and useful way, but they also instruct the software to make coding (mathematical) linkages as well. All of this convenience comes at the cost of processing speed for the final simulation.

FORTRAN, other coding languages, or mathematically-orientated platforms such as *MatLab* (mathworks.com) will run the code much faster, though at least for initial construction and deployment (the subject of this book) actually watching the model running can be extremely valuable (not least for locating errors), and the final code can be transferred for execution in a faster language relatively easily as required.

The choice is yours. Use whatever you find most attractive to you. Do not let snobbery put you off any particular platform; the only thing that matters is that the model itself and the software platform are fit for purpose.

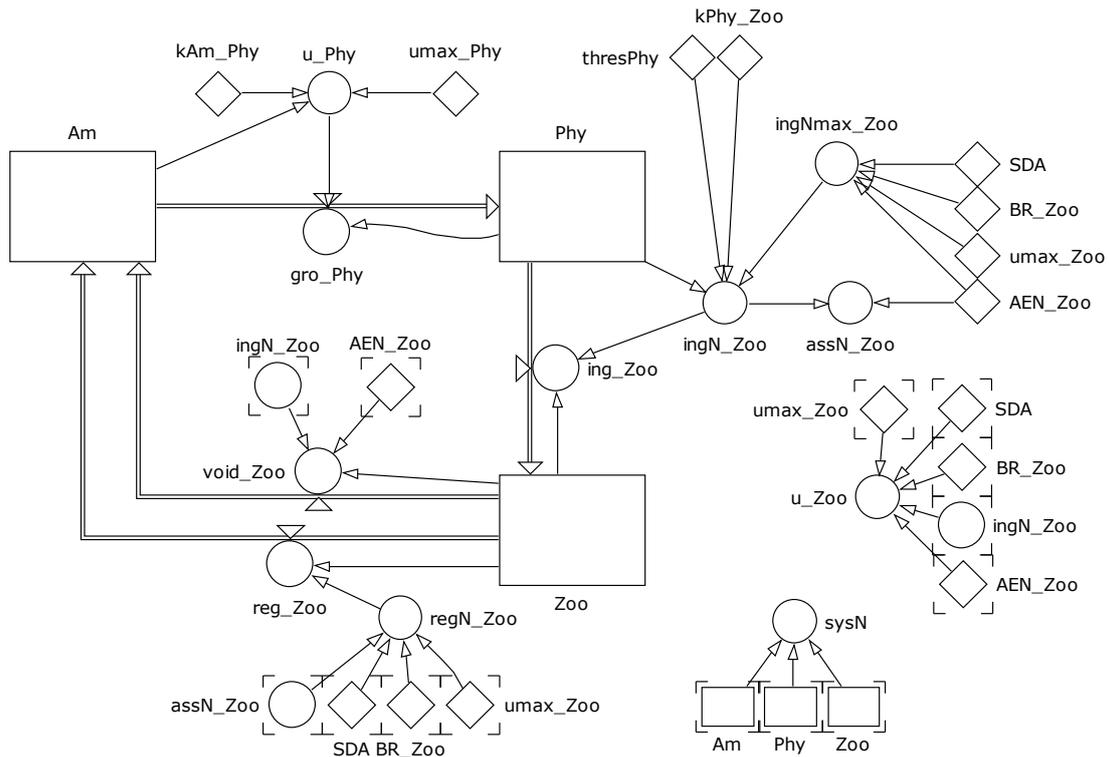


Fig. 2.2 A Forrester diagram representation of a simple systems dynamic predator-prey model. Flows of material (here, as nitrogen) between the state variables (boxes) are indicated by pipelines with their direction shown by the arrowhead. Auxiliaries are indicated as circles; note that the flows (pipelines) are described by auxiliaries shown attached to the pipeline as a valve, or tap. Constants are shown as diamonds. A thin arrow leading from a symbol indicates that the numeric values of that variable is used in the equation defining the arrowed variable; most auxiliaries have connections from several other variables. Symbols with corners are copies (snap-shots) of symbols used elsewhere in the diagram; if this approach is not used the diagram would resemble a plate of spaghetti! This particular model is developed in Chapter 5.

2.8 Deterministic vs Stochastic Models

The models considered in this book are deterministic – every time you run the model with the same input variables, you will get the same outputs. To introduce a level of variation, you need to vary the input variables. This can be achieved by making some inputs and constants random numbers, perhaps centred on a mean with a stated standard variation. This can be undertaken automatically by the software as part of a dynamic risk analysis (see Section 2.12 and Chapter 13). That analysis is often conducted to test the model structure, but the very same analysis, run in a model that has been accepted as being fit for purpose, will report outputs with at least some component of stochasticity. You can also run the model with links to a random number function in the software.

Of course events in nature may not accord with those in a simulation not simply because of stochasticity in nature (notably related to the weather) versus the deterministic form of the model, but in reflection of the model missing structural components (physiological processes,

functional groups etc.). Arguably “stochastic” can also be used as an excuse for a lack of understanding or (mis-) representation of the system.

2.9 Functional Types, and Biomass vs Agent- or Individual- Based Representations

Real organisms are individuals and each is, in subtle ways, unique. Even cells that are clones will be in different biochemical and cell-cycle states at any instant in time, and they will be in different physical locations and thus exposed to different conditions. Models, being simplifications, cannot represent the full activity of all individuals; some level of grouping is required. And of course in practical ecology the status of an organism type is determined by averaging across many dozens through to, for smaller microbes, many millions of individuals. In plankton ecology the situation is often even more complex. For example, a sample for measurement of plankton C-biomass can only be fractionated readily according to particle size and will thus contain many organism types each with different physiological states and growth rates, etc., and of different trophic level.

It is interesting here to note the contrast between mathematical ecology and molecular ecology. While molecular biology gives us tools that enable us to subdivide organisms and individuals, mathematical approaches do (or force) the converse, and thus merge individuals and groups.

Organisms in ecology may be merged into **functional groups**; these are organisms that play similar roles in ecology (with respect to trophic dynamics). In the context of plankton, such groups may be termed **Plankton Functional Types** (PFTs). Some may ascribe PFT according to biogeochemical functionality (e.g., calcifying, silica-depositing or N₂-fixing species). However, such biogeochemical functionality is actually a function of ecology; organisms do not evolve to undertake what humans may view as a biogeochemical activity (see Flynn et al. 2015).

Most plankton models are biomass based, with their state variable in units of, for example their C-biomass, as mgC m⁻³. Any description of organism numeric abundance is then calculated with reference to the average mass per individual. There are instances, however, where tracking of individuals is important, for example of subpopulations migrating vertically in the water column. Recognising the sheer number of planktonic individuals (often many tens of millions per m³), so-called “**individual based models**” (IBMs) are invariably actually “**agent based models**” (AGMs). Similar approaches are used for models describing fish migration, for example. Each “agent” represent many individuals. Sometimes such agents are termed “super-individuals”, not because they are super in a genetically-modified-organism sense, but because many thousands, perhaps millions, of real individuals are represented as a single cohort, accorded the same physiological status, centred on a common location in space, growing, dying, sinking, swimming etc., all in synchrony.

Pragmatically there is a very good reason for taking this agent-based approach. Simulations of the movement of smoke particles in the air, or of clay in a water column are relatively simple compared to the challenge of describing biological activity at the individual level. Inert particles do not grow, multiply, die or be consumed and converted into a myriad of voided faecal particles. Computationally to keep track of every particle is thus much easier if the number of “particles” is known (and can thus be set) at the beginning of the simulation. The “particle” refers to a collection, a cohort of individual organisms in a given space; the population changes because the cohort changes in size.

The use of IBMs provides additional opportunities and challenges. For microbes (prokaryotes and most protists) there is *de facto* only one body form which grows to a critical size and then splits into two. For metazoan it is very different. For fish there is a transition from a planktonic egg, to planktonic juvenile stage that gradually grows to become an adult; the body plan is broadly similar once beyond the first-feeding stage. For mesoplankton, such as copepods and krill, there are distinct stages of the life cycle which may require an elapsed period of time and a gain of so-much body weight (weight-at-age) before transition can occur to the next stages. Progression can be halted or indeed death can occur if this process does not proceed according to the biological clock. To simulate this requires the modeller to make additional considerations concerning how to progress IBMs from stage to stage. An example of such a model and its deployment is given in Flynn & Irigoien (2009); we will not consider them further in this book.

2.10 Dimensions in Space and Time

Changes in spatial distributions of organisms and resources are critical features affecting ecological dynamics. In theory at least, every organism and resource could be assigned a position in space with respect to x,y,z coordinates set against some reference point (most obviously, latitude and longitude). Depending on the system being considered, there is then the challenge of describing movement and behaviour relative to other components in the system (resources, predators, physical features).

The easiest way to include space is to describe the presence of organisms as a concentration (numeric or biomass density); this is the route taken in this book. The caveat is that we assume a homogeneous distribution in the space considered. Thus, organisms are assumed to equally distribute themselves, or physical processes such as water movement mix the organisms, throughout the space in question. Even in models with detailed high resolution spatial structures, the coordinates of each zone inevitably encompass a portion of space of perhaps 10s m, or km dimensions. Just as so called individual based models (Section 2.9) actually describe cohorts of organisms assumed to be behaving in unison, so the spatial descriptions operate at a specified grid scale. Within that grid, organisms are again considered as being homogeneously distributed. Over time, a proportion of organisms and (as appropriate) resources may be moved between adjoining zones.

At the simplest level, a model of ecology can be operated at steady-state (*de facto*, with no time dependency) and with no explicit description of space (i.e., zero dimension; 0D). A simulation by definition involves time dependency, so we do not need to state a dimension for time in a systems dynamic model; a 0D simulation is thus one in which space is not considered. An example of such a 0D simulation would be if we consider a dynamic model of activity within a homogenous mixture of organisms and resources, such as within a culture flask or a well-mixed pond.

Simulations of terrestrial systems may be 0D, 1D (a linear transect), or 2D, or if we consider surface topography such as hills, perhaps as 3D. An aquatic system may obviously be 3D (full x,y,z). There are also simulation models that some workers describe as “½ D”, with the vertical water column split into an upper mixed layer, and a lower unmixed layer; we will consider such a model in Chapter 12.

Describing simulations operating beyond 0D involves partitioning space into areas or volumes. At its simplest these could be handled as a grid of squares or cubes, though triangles and pyramids

give greater scope for defining irregular space. The calculations, in what is commonly termed finite element modelling, are computationally expensive. At each time step there is an exchange of materials (biomass, nutrients, etc.) between adjoining grid cells. Just moving non-living materials around is challenging enough, and high simulation resolution demands small grid dimensions together with small integration step sizes. Add in the complexity of biology, with organisms multiplying, dying, degrading into parts etc, and the computational load rapidly rises so that you need a high-performance computer to proceed effectively.

The models described in this work are all operated as simulations (i.e., with time) in 0D, or at most $\frac{1}{2}$ D. No simulation of ecology should be placed in a more complex scenario unless its behaviour within 0D is understood and found to be acceptable. In this book emphasis is placed on achieving that goal, of producing sub-models for biological components that are fit for purpose, which could then be placed with confidence within a more complex spatial description.

2.11 Initial Checks

There are several simple checks that should always be undertaken during the construction and testing of SDMs, and indeed of any model. These checks should be repeated under different simulation conditions to ensure the model is robust (i.e., it does not “crash” or otherwise misbehave).

First though, you need to visualise the model output.

Data visualisation

Models generate a lot of data. If you consider the model shown in Fig. 2.2, which is not a complex model in relative terms, you will get a feel for the permutations available; it may well be instructive to consider plotting every auxiliary and especially every state variable. Most obviously you will plot simulation output against time. As far as possible it is a good idea to co-plot related data series on the same graph. Thus, from Fig. 2.2 it would be logical to co-plot the state variables, and also the sum of those values (*sysN* in Fig. 2.2). Plotting response stimulators against the response, on x-y scatter plots, is useful if only to check your equations are doing as you expect.

Other x-y scatter plots, coupled with plots of changes in relative proportions of data upon time-plots, are useful for gaining a better understanding of factors affecting the dynamics. For example, a plot of prey (*x*) vs predator (*y*), and of predator:prey vs time show how a the system output evolves towards what is termed **an attractor**. An attractor is a space in model output towards which the dynamics will always move for a given set of input variables (e.g., see Fig. 2.3). The model may settle to a specific equilibrium position (an attractor point), or to a delimited range of output (an attractor basin, where a quasi-equilibrium is attained).

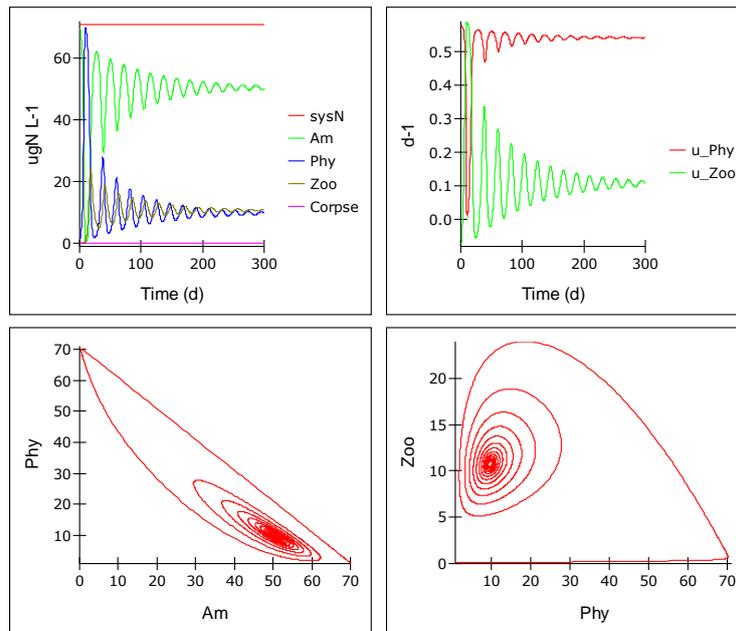


Fig. 2.3 Output from a predator-prey model showing how over time the oscillations in ammonium (*Am*), phytoplankton (*Phy*), zooplankton (*Zoo*) and corpses (*Corpse*) dampen over time. The relationship between resource and consumer (*Am* vs *Phy* and *Phy* vs *Zoo*) can be seen to spiral in towards their respective attractor points. The model generating these plots is described in Chapter 11.

Certain parts of a system may display high sensitivity to changes in input variables. When such variables are changed, the attractor can shift to a different space in model output. This is termed a **bifurcation**. In a real ecosystem, bifurcations can be associated with so-called tipping points, where the ecology changes to a different state from whence it may be difficult to revert back to the original state. Whether your model properly describes reasons for tipping point behaviour depends on how closely the model describes reality. In the model developed in Chapter 17, slight changes in palatability of the prey with nutrient availability dramatically changes model behaviour; if the prey are not grazed then nutrients are not recycled so the prey become even less palatable, and so on.

Different graphing approaches play a crucial role in visualising model behaviour. And the more complex the model the more complex are the permutations of visualisation. For example, 3D plots can be most revealing of processes controlling the dynamics, especially if you can rotate the plot to better interpret it.

Whatever plots you use be very careful not to use automatic scaling options by default. Automatic scales have their uses, but they can also readily present a distorted view of the data.

Checking units:

Whatever is done with numbers must also be done to units. Thus, while variables with different units may be subjected to multiplication or division, such variables cannot be subjected to addition or subtraction. The latter has immediate and important consequences; flows of material between state variables (e.g., nutrient \rightarrow plant \rightarrow animal \rightarrow nutrient) thus require that all these state variables must have the same unit, and the flows will have the same unit multiplied by 1/time. Thus in a model, foxes do not feed on rabbits; there is a flow of rabbit-C, or rabbit-N, into fox-C, or

fox-N (respectively), and the rates of flow are thus of $C d^{-1}$, or of $N d^{-1}$ (assuming time is in days). It is worth noting the practical implications of this for biologists and ecologists; merely counting organisms is not sufficient to support systems dynamic approaches.

Mathematic overrun and other errors:

The first occasion a model is run, more than likely it will do something that is undesired.

The first thing to rule out is the presence of fatal flaws that lead to gross mathematical errors, such as generating values of variables which are positive or negative infinity. And the first thing to try to solve this problem is whether decreasing the integration step size (or perhaps changing the integration method) corrects, or at least decreases, the magnitude of the errors. In general, when first testing a model it is best to use a smaller step size than is strictly necessary. This is demonstrated in Chapter 4.

The most common problem beyond this stage are of values exceeding sensible bounds due to mathematical/processor errors or conceptual/structural errors. The most common mathematical/processor errors are associated with computing positive or negative infinity; the most common cause is a “division by zero” event, which generates infinity. Conceptual/structural errors result in a parameter value exceeding its logical bounds, such as becoming negative (though this can often be an indication of an integration error, such as using too large a step size), or a quotient exceeding the bounds of 0 to 1. In all instances, the first challenge is locating the problem, and the second is preventing its occurrence.

To locate the problem first requires that the model is interrogated at the time-steps immediately before that at which the error is flagged in state variables. This is because the calculation giving rise to the error (e.g., $1/0 = \text{infinity}$) will have been generated in an auxiliary or flow, and not in the state variable itself. The allied auxiliaries and state variables feeding values to the equation then need to be checked to locate the offending input.

Sometimes, especially in complex models, isolation of components of sub-models is required. (Needless to say, you should only ever interconnect sub-models that have individually been tested thoroughly.) Thus in a food web model it may be desirable to take a predator off-line to locate a suspected error elsewhere, or for example to confirm the problem is at the interface between the predator sub-model and other components. Rather than setting the state variable defining the presence (biomass) of that component to zero, it can often be safer to set it at a very small number (e.g., $1E-100$) and also to set its accompanying rate of increase (e.g., the constant defining the maximum growth rate) to a similar very small number. This is because setting input variables to zero may (depending on the equations) trigger a division-by-zero error to add to the pre-existing problems.

Whatever you do in trying to track problems, be sure to document the steps so that you can reverse them when the time is right. You may also wish to save the file as a new name before undertaking the correction attempt.

Next, you need to prevent the problem. Structural errors can require anything from a radical rebuilding of the model, through to the more mundane correction of equation structure. The most common error in equation construction is misplaced parenthesis (“brackets”); this is a particularly easy error to introduce when transferring equations from traditional mathematical notation to the required linear text style needed in the modelling programme. In general, equations in this book

are given as linear equations similar in syntax to those entered into spreadsheets or most modelling and coding platforms.

Division-by-zero errors can be prevented either by altering the equation syntax, or if that is not readily achieved, simply by adding a suitably small number (e.g., 1E-100) to the denominator. Preventing values going negative, when they should not, can be trapped using logical tests (e.g., “only do this if the parameter value is positive and less than 1”). Neither of these approaches should be used to compensate for otherwise sloppy equation work or poor choice of integration protocols (see Section 2.6). Such traps remain, however, pragmatic solutions for preventing occasional misbehaviours. This can be particularly useful when leaving a model to run many hundreds of simulations automatically using random-generated input values for dynamic sensitivity analyses (Section 2.12, Chapter 13).

System balance:

A systems dynamic model must not simulate spontaneous production or loss of material. In essence, the simulation must obey the law of the conservation of mass. Thus, in our example above, the total sum of nutrient-N plus grass-N plus rabbit-N plus fox-N must remain constant throughout time. In Fig. 2.3 it can be seen that system-N (*sysN*; top left panel) remains constant despite the oscillations in the values of the state variables. It is important when conducting this check to set at zero any flows describing input and outputs of material beyond the system being simulated.

This check is easy to do, and should not be overlooked.

There are two obvious explanations if this check fails: the conceptual basis of the structure of the model is incorrect, and/or the mathematical basis of the simulation is incorrect. If the structural basis is incorrect then this manifests as a failure to account correctly for all flows in and out of all state variables. If the mathematical basis is incorrect (and assuming that other checks have been satisfied) then usually an error in integration step size, or perhaps in integration method, is implicated. The first thing to try is to halve the step size, taking note of the behaviour of the model, and of the numeric value of state variables at given times during the simulation. If after repeatedly cycles of halving the step size the system still does not balance then most likely there are errors in the structural basis of the model.

It is important to note that the system balance will never remain exactly the same, to the umpteenth decimal position, because of cumulative errors in computer operations. What is being checked for here is some systematic error – usually failures are quite obvious but not necessarily apparent under all conditions, so system balance checks should be made under various operating scenarios. These include operating the model with different combinations of input values (e.g., initial organism abundance nutrient status, activity rates etc., light, nutrient concentrations). It can take considerable effort, and patience, to locate structural errors in large models. It is best to build smaller sub-models (such as one for each function group of organisms) and check them individually before bringing them all together and checking the whole model.

2.12 Sensitivity Tests

This is a check of model structure, to ensure that the control of events has not unwittingly been made overly sensitive. Over-sensitivity, for example in feedback loops, may not only indicate failings in the conceptual basis for the model, but also require the deployment of very small time-steps to ensure that high accuracy is used in the integration routines. For most biological and ecological systems we know very little with any detail, and even less with any precision; there are typically large margins of doubt around values of input variables controlling the dynamics. In addition, most often what is modelled are functional types (e.g., all phytoplankton) and not just a strain of a species; in consequence there cannot in reality be a single fixed maximum growth rate value, for example. It makes good sense, then, to make models that are not overly sensitive to the estimate of these constants. By over-sensitivity we refer to an event such as a doubling of an input variable alters the output 10 fold.

There are two types of sensitivity test that are readily used in SDMs. One considers a single input variable (constant) in a model running to what is termed “steady-state” and the consequences upon model outputs. The other is a multi-constant dynamic test, sometimes called a **risk analysis**. These tests should be conducted sequentially.

In the single constant test the model, or more usually some section of it, is run under steady-state (i.e., the values of state variables around the component being explored become invariant) and the input variable (constant) being considered is halved or doubled. The effect of this halving or doubling is monitored on the components; a good result (i.e., not unduly over-sensitive) is if output values alter broadly pro rata with changes in the input value; thus when the input is doubled, the outputs also double, or perhaps halve. A bad (overly sensitive) result would be if on doubling the input variable the output altered 10 fold.

The multi-constant test gives an insight not only into how individual components operate but also into how the whole system works; there may be good acceptable reasons (e.g., associated with cascade events, and the removal of a key-stone species from a food web) why a complex system describing the interactions between many organisms may be sensitive.

If the model is overly sensitive then it may be necessary to revisit the model structure (Fig. 2.1).

Sensitivity analyses are explored in detail in Chapter 13.

2.13 Tuning and Validation

Tuning is a process through which the values of model constants are altered to best align model output against a reference data set. Thus, for example, maximum growth rates and prey-preference values may be changed. If through tuning the behaviour of the model cannot be brought into an agreeable level of alignment with the reference data then it may be necessary to revisit the model structure (Fig. 2.1).

Validation is a process where a model that has been tuned against one data set is compared in its behaviour against another data set. For example, having tuned the model for phytoplankton growth in a 0.5L flask with a nutrient concentration of 50µM ammonium, how does the output compare against a data set from an experiment conducted in a 10L bioreactor containing 250µM

ammonium? Again, if an agreeable level of alignment is not obtained, it may be necessary to revisit the model structure and tuning.

These processes are considered in detail in Chapter 14.

2.14 Concluding Comments

Biology and ecology are immensely **complex adaptive systems**, or more appropriately termed, complex acclimative systems (adaptation being an evolutionary process, which in contrast to acclimation is typically not reversible). Even the simplest SDM directed at such systems can appear complex. The learning curve is steep but just attempting to build models, let alone running the product, is invariably informative. A dynamic model that does what it should do is an extreme test of our understanding.

3. Naming Variables and Building Third Party Models

Terms and concepts introduced in this chapter- naming conventions, transcribing 3rd party models, plagiarism

3.1 Algebra and Names for Variables

Mathematical models are built around algebra, and algebra is based upon “sentences” made of mathematical symbols or names, together with mathematical operators. The symbols or names collectively are “parameters” (if their value is fixed) or “variables” otherwise. For brevity, in what follows we shall refer to them all as variables.

While simple sets of algebraic equations contain few variables, most dynamic models in total contain many dozens, perhaps even hundreds of variables. And that is before you start to combine sub-models describing (in the context of this book) different plankton types. Invariably there are far too many variables to name relying upon just single letters of the alphabet. In consequence, you will need some form of naming convention otherwise as time goes by you will be in danger of losing track of names, what they mean, and you may also start reusing names in contrary situations. Of course, you could give each variable a full descriptive name, and many software platforms will allow you to do so. In practice though you need to strike a balance between names that are long enough to help you recall what they refer to, versus short enough not to make viewing the equations unwieldy.

3.2 Naming Variables

The name given to each variable in the model code needs to be unique, ideally short and informative, and achieved typically (depending on the software) using only standard letters of the alphabet and numbers, and most usefully also the character “_”. These requirements contrast with traditional mathematical equation formats, which may often include the use of Greek characters and super- and sub- scripting. You cannot typically use either Greek symbols or super/sub –scripts in coding platforms. Equations are also usually entered in linear form, and not in a traditional mathematical format.

All of this can prove quite restrictive if not confusing or indeed simply annoying, especially if usages of the same name contrasts between models and/or author. It is particularly problematic when models are described in the literature making extensive usage of traditional mathematical notation with Greek characters as this immediately drives you to invent your own naming conventions before you can commence rebuilding the published model (see Section 3.5).

There are no hard and fast conventions for assigning names, other than some level of logic or tradition. Names cannot use terms reserved by the software platform, such as mathematical functions (e.g., you likely cannot use “LOG”, or “log”, to describe tree logs, as this name is reserved for the mathematical function *logarithm*).

For the types of models described here, for plankton, certain characters should logically be reserved, notably those for elements (e.g., *C*, *N*, *P*, *Fe*, *Si*), and physical parameters (e.g., *g* for

acceleration due to gravity, T for temperature, $PF D$ for photon flux density, z for depth). The character “ u ” is often used to donate the Greek letter μ (yes, the lower case Greek letter “ m !”).

Upper and lower case characters may be used to aid interpretation of the variable name. However, as software may not differentiate between upper vs lower case, to help others to use your model code within their own software platform it is safest to assume there is no functional difference between cases.

There is a consequence of using variable names exceeding 1 character, and that is to remember that an explicit multiplication symbol is required when writing equations. Hence $PF D$ does not mean $P \times F \times D$; $PF D$ is a name for one variable (actually, here, as *photon flux density*). When writing equation including multiplication you need to either use “.” (note this is not the same as the decimal point, “.”) or “ \times ”, or “ $*$ ” (which is the symbol most likely used by the software platform itself). So, Einstein’s famous equation, $E=mc^2$, would be written as $E=m*c^2$, or perhaps $E=m*c**2$.

3.3 Naming Conventions

As a convention I will (as far as possible) use the following format for naming variables for entry to modelling software:

{Primary Name}{With respect to}_{Owner}

In traditional mathematical syntax this may be written this as:

Primary Name^{Owner}_{With respect to}

Thus, the maximum growth rate for zooplankton would be written as:

u_{max_Zoo} or in traditional format as: u_{max}^{Zoo} or as: μ_{max}^{Zoo}

The C:N ratio for diatoms, would be written as CN_Diat , or CN^{Diat} . If it was necessary to identify C:N as a mole ratio rather than a mass ratio, then we could use:

CN_{mole_Diat} vs CN_{mass_Diat} or CN_{mole}^{Diat} vs CN_{mass}^{Diat}

As far as possible I have tried to preserve a unique usage of each variable name. On occasion this creates conflicts with the names of some classic models and their components. Thus in Chapter 12 we consider the “*nutrient-phytoplankton-zooplankton*” model, usually referred to as the “NPZ model”. Using the above naming convention this could be interpreted as the “*nitrogen-phosphorus-depth*” model! We could rename this as the “NutPhytoZoo” model which, while it does not trip off the tongue so readily as “NPZ”, is perhaps more informative and certainly less ambiguous.

3.4 Variable Name Formats used in this Book

In the textual descriptions I have sometimes used the traditional format (e.g., u_{max}^{Zoo}) as this is more compact and hence it is easier to see how the equations fit together. I have also sometimes used additional (superfluous) levels of parenthesis in equations where doing so helps the reader understand the linear version; missing levels of parenthesis is a major cause of error in model building, and especially in transcribing equations described using traditional mathematical syntax into the linear equations required by most modelling software platforms.

In the tables, which describe each variable, equations are given in a linear form suitable for copy-pasting into modelling software. While you still need to check that the equation has been copied in its entirety, this approach should minimise the effort and the risk of introducing errors.

So for example, in the text, the equation:

$$u^{Alg} = u_{max}^{Alg} \cdot \frac{Am}{(Am + k_{Am}^{Alg})}$$

would be written in the accompanying tables as:

$$u_Alg = u_{max_Alg} * Am / (Am + k_{Am_Alg})$$

While every effort has been made to syntax check all equations, those in the tables should be considered as definitive as these have been directly copied from operational models. (See also "Please Read Me" for additional comment concerning updates.)

3.5 Rebuilding Published Models

Almost certainly at some point you will wish to rebuild someone else's models. Invariably your first challenge will be to convert the original names of variables into names consistent with your own needs.

It is recommended that you transcribe the published model into a spreadsheet, with separate columns for the original variable names, for the original units and for the equations or values. In the adjoining columns you can then enter the name you will use in your reproduction, your chosen units, and then your version of the equation with reference to all the revised variable names. Do not forget to document the description of each variable, as this gives the explanation as to what is actually happening in that equation.

Check carefully that the units all balance. Be particularly vigilant for instances where transforms, such as $\times 10^3$, are missing from published equations. You may only be alerted to such instances by a mismatch in units (e.g., $\mu\text{moles L}^{-1}$ rather than mmoles L^{-1}). Watch out also for changes in base units, such as cm to m, and in time from s to d.

All of this can be a tedious, and not infrequently a frustrating task; that is especially so if variables are not described fully in the source publication. It is however very important that you complete the task, cross checking that units of auxiliaries match those emerging from the transcribed equations etc., before attempting to actually build the model.

Published models often lack basic information such as the time-step and integration routine type. See Section 2.6 and the example in Chapter 4 (Section 4.9) for guidance.

3.6 Giving Credit Where Credit Is Due

Model structures constitute intellectual property, covered by copyright. Changing parameter names does not disguise the underlying conceptual basis. So, if you replicate someone's model, or use some of their concepts, then you must acknowledge the original authors. To copy another person's work and pass it off as your own is **plagiarism**. This applies to reproducing descriptions of sub-components as much as to using the complete model but perhaps operating it in a different scenario. Thus, if you have used the predator model from a given source coupled with your own prey description, you still need to acknowledge that you have adapted the work of another author. Apart from the fact that you must do this, it can be to your advantage in another way, because you can also reference any checks that the original authors have made (sensitivity, tuning, validation) and thus add credence to your total construct.

4. A First Model – Nutrient-limited Growth

Terms and concepts introduced in this chapter- conceptual models, response curves, Monod equation, specific growth rates, chemostats, dilution rates

4.1 Ecological Context

In nature, very many factors change simultaneously, thus confounding interpretation. A common driver in experimental biology is the notion of changing one factor at a time, and seeing what happens. In experimental physiology, responses to resource (nutrient or food) limitation represents a popular arena for research, there being 10000s of publications on the topic ranging from very specific detailed empirical investigations to generalised theoretical studies of competition for different resources. Here we consider nutrient-limitation of phytoplankton growth. As we shall see (Chapter 8), in practice it is actually all but impossible to investigate a single-nutrient limitation because of feedback processes linked to organism abundance, but with models you can do (almost) anything. (The important caveat is, should you?!)

4.2 The Conceptual Model

All models start as a concept. In the context of ecological models such a concept will likely be akin to a food web diagram, with boxes or other symbols denoting organisms and resources, and arrows indicating flows. For detailed models of ecophysiology, the conceptual model may appear similar to a biochemistry pathway diagram.

The concept here simply describes the growth of a nutrient limited phytoplankton population. The nutrient will be stated as ammonium-nitrogen. Respectively, let us name the phytoplankton as *Phy* and the ammonium as *Am*. The identity of the phytoplankton need not concern us at this point; all phytoplankton can use ammonium (noting that high levels are often toxic, so we should keep the concentration below the equivalent of ca. 100 μ M). From Chapter 2, we will recognise that *Phy* and *Am* must be state variables; they are tangible quantities that have a history.

The next matter to consider is the form of the **response curve** describing limitation of the growth of *Phy* by the availability of *Am*.

4.3 Response Curves

Interactions, or causal relationships, between factors (such as between nutrient concentration and uptake, between gut satiation and the cessation of feeding) can be described using **response curves**. Response curves are usually visualised with the stimulus or controller (independent variable) on the x-axis, and the effected (dependent variable) process on the y-axis. Each of stimulus and effector may vary over a fixed range (e.g., 0 to 1), or over an open range (e.g., 0 to some stated or perhaps unstated value).

Fixed range response curves are particularly useful when both stimulus and effector are described as quotients; quotients are numbers that ranging from 0 to 1. In this manner both stimulus and

effector are normalised, with their ranges running from a minimum (0) to a maximum (1). An example would be the relative rate of satiation (% fill of the gut) to the relative rate of feeding (% of maximum rate).

Here, for the description of growth of a nutrient-limited phytoplankton populations, an open response curve is appropriate. This is because the concentration of the nutrient (the substrate for growth) may vary over a wide range, accepting that nutrient concentration is ultimately limited by solubility. The y-axis describes the rate process, which will be limited by cellular metabolic processes.

We will come to the equation itself shortly. For now, we just need to appreciate that the response curve may be expected to resemble a saturating curve of the form shown in Fig. 4.1. Such a curve may also be termed a type II response; type I is linear, and type III appears as a sigmoidal (“S”-shaped) curve. This particular curve, in Fig. 4.1, is a rectangular hyperbola and it will crop up as the basis for a response curve on numerous occasions.

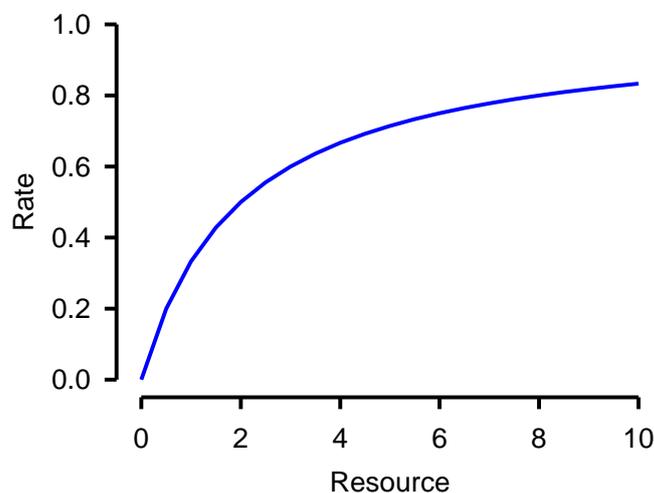


Fig. 4.1 Form of rectangular hyperbola relating resource availability to process rate.

4.4 Assigning Variables

We can now construct the conceptual model as a diagram and start to assign parameter types and units. Firstly, we identify the state variables and the flow between them. The state variables are the nutrient ammonium (Am) and phytoplankton (Phy). And there is a flow of material from nutrient concentration to the phytoplankton biomass supporting population growth; let us term this gro_Phy . Our conceptual model thus looks like Fig. 4.2, and we now need to define gro_Phy .

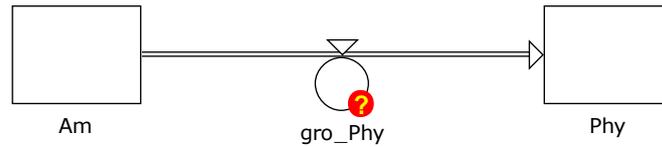


Fig. 4.2 Conceptual model base for phytoplankton (*Phy*) growing using ammonium (*Am*) as the limiting nutrient. This is a Powersim Studio Forrester diagram representation. The “?” indicates that the equation defining the variable for phytoplankton growth rate (the auxiliary *gro_Phy*) has not been configured yet. This auxiliary will define the flow of material (nitrogen) along the pipeline (arrow) between *Am* and *Phy*; it is attached to the pipeline via an inverted triangle indicative of a valve controlling the flow.

We know that the units of both state variables connected by a flow must be the same, and that the flow will have the same unit as do the state variables, but (as it describes a rate) expressed per time unit. Nutrient concentration (and we have defined this nutrient as ammonium), could logically have either mole or mass units per volume. If we were to consider growth of a culture of phytoplankton in a flask, then L would be a logical unit of volume. Accordingly, the nutrient concentration could be M (molarity) or g L^{-1} . The phytoplankton biomass must have the same unit; this cannot be as M (the biomass is not dissolved in solution; it is particulate), so the units must be either moles L^{-1} or g L^{-1} . For this model, let us go with units of mass (i.e., g L^{-1}). Pragmatically, ammonium concentrations in experiments would likely be in the $\mu\text{gN L}^{-1}$ range; a quasi-natural concentration of ammonium may be in the $10 \mu\text{M}$ range, which is $140 \mu\text{g ammonium-N L}^{-1}$. So, let us define the units for both *Am* and *Phy* as $\mu\text{gN L}^{-1}$.

It is worth noting, in passing, that the units for phytoplankton are not as cell abundance, as an experiment biologist would most likely determine. If we wished to describe changes in cell number we would need a transform to convert the biomass concentration ($\mu\text{gN L}^{-1}$) to cell abundance (cells L^{-1}); that transform requires knowledge of the average N content per cell (see Section 4.8).

The flow of N between *Am* and *Phy* (*gro_Phy* in Fig. 4.2) is not a fixed rate, but varies both with nutrient availability (*Am*) and with the size of the phytoplankton population (*Phy*). The rate will thus be described by an auxiliary. We need to define the flow by an equation, or equations, linking *Am* and *Phy* and the growth rate of *Phy*. The time unit for the simulation we are considering would logically be day; this is because the minimum doubling times (equating to maximum growth rates) for these organisms are of the order of ca. 0.25 to 2 doublings per day. So the flow of material between *Am* and *Phy*, which is *gro_Phy*, has units of $\mu\text{gN L}^{-1} \text{d}^{-1}$.

The value of *gro_Phy* describes the growth rate of the population. It is important to note that this is not the growth rate of components (individuals) of the population. To understand why not, let us return to the response curve (Fig. 4.1).

The response curve (Fig. 4.1) relates growth rate (let us call this parameter *u*, equating to Greek μ) of the individual to the availability of the nutrient. The growth rate ranges from 0 (with no nutrient available) to a value at high nutrient availability that is close to a maximum value, which we can call *umax*. A plausible value for *umax* is 0.693d^{-1} ; this value equates to a doubling time of 1 day assuming asynchronous growth of the members of the population (see Section 4.5). For application to the

phytoplankton in our model, let us call these variables u_Phy (actual, current, growth rate) and $umax_Phy$ (maximum growth rate).

The full units here for u_Phy and $umax_Phy$ actually describe an increase in phytoplankton-N per g phytoplankton-N per day, which we write as $gN\ gN^{-1}\ d^{-1}$. This describes growth as an event similar to compound interest in a bank account; every g of biomass that is synthesized contributes to the building of the next g of biomass. The full description for this rate in the model we are building is the “N-specific growth rate”; the “gN” units cancel out, leaving just d^{-1} . Typically, however, this is referred to as the **specific growth rate**, but without stating what it is “specific” to!

4.5 Specific Growth rates, Chemostats and Dilution Rates

The term “specific growth rate” crops up frequently in the literature, usually with little elaboration. It is calculated from experimental data according to the following equation:

$$u = \frac{\text{Ln}(x_{t1}) - \text{Ln}(x_{t0})}{(t1 - t0)} \quad \text{Eq.4.1}$$

Here x is the value of the variable (e.g., cell number, biomass) measured at times $t0$ and $t1$. Noting that subtracting logs (here, as the natural log, Ln) is akin to division, the units of x cancel out, and we are left with the unit for growth rate, u , as simply time^{-1} .

And herein lays the problem; because the units of x cancel out, the unit upon which the rate is “specific” is often not always recorded. And it really should be. Indeed, it is always best to state the specificity of the value. The reason for this is that rates described as ..

cell-specific (e.g., $\text{cells cell}^{-1}\ d^{-1}$),

C-specific (e.g., $gC\ gC^{-1}\ d^{-1}$),

Chl-specific (e.g., $\text{moles Chl (mole Chl)}^{-1}\ d^{-1}$),

or

N-specific (e.g., $gN\ gN^{-1}\ d^{-1}$)

.. are not necessarily of the same value.

In fact they will only be the same in a homogenous suspension of a strictly asynchronous culture (i.e., a well-mixed suspension of organisms all at different stages of their life cycle), growing at **steady-state**.

By definition, **growth at steady-state** requires that, on average across the population, all components within an organism are changing at the same rate, such that (as we have just considered) specific growth rates determined by any and all means report the same numeric value. Such conditions are only likely to occur in reality within a culture environment such as an established **chemostat**.

A chemostat is a culture system (operated usually in a flask), in which the volume of culture is held constant while liquid is pumped in and out of the system; fresh growth medium is pumped in and at the same rate culture medium containing residual (unused) nutrients plus organisms are pumped

out. In such a system, when running at steady state, the dilution rate defines the specific growth rate of the organisms. We will explore chemostat operations and dilutions further in Chapter 7.

As for the magic number, 0.693, this is $\ln(2)$ and it is the growth rate that equates to a doubling per time unit; thus growth at a rate of 0.693 d^{-1} equates to a doubling in biomass per day. The reason that the number is not 1 is because growth is considered to develop in a way akin to compound interest; every fraction of time sees another addition to the biomass and the new total biomass contributes to the building of new biomass during the next fraction of time. And so on. Two doublings a day would give a value of u of $2 \times 0.693 \text{ d}^{-1}$; a doubling every other day would be $0.5 \times 0.693 \text{ d}^{-1}$.

4.6 Relating Nutrient Concentration to Growth Rate

Let us return to our model, which for simplicity we assume is describing biomass growth in a continuously illuminated system (see Section 4.11 for caveats). The response curve will return a value of u_{Phy} , as the N-specific growth rate for a given concentration of ammonium. Recall the full units of u_{Phy} are $\text{gN} (\text{gN})^{-1} \text{ d}^{-1}$; however, this is not the unit of the population growth rate (gro_{Phy}), which is $\mu\text{gN L}^{-1} \text{ d}^{-1}$. The value u_{Phy} is the growth rate per unit of phytoplankton biomass (for which the units collapse to just d^{-1}), and we have $\mu\text{gN L}^{-1}$ units of biomass (Phy).

The population growth rate, gro_{Phy} , is thus given by $u_{Phy} \times Phy$. Recalling that whatever we do with the variables we do to the units, then the units of gro_{Phy} will be:

$$(\text{gN} (\text{gN}^{-1}) \text{ d}^{-1}) \times (\mu\text{gN L}^{-1}) = \mu\text{gN L}^{-1} \text{ d}^{-1},$$

From Section 4.4, this is what we expected.

We thus need an auxiliary to describe u_{Phy} , in addition to that we have already identified (gro_{Phy}), which describes the flow of N from ammonium (Am) to phytoplankton (Phy).

The response curve used for this relationship is expected (based on decades of usage from the 1940's work of Monod, 1949) to take the form of a curve resembling that of a rectangular hyperbola. The equation for this is simple, and you may recognise it as also being the same as that used as a simplified description of enzyme kinetics (termed the **Michaelis-Menten equation**).

The generic form of this equation is:

$$V = V_{max} \cdot \frac{S}{(S+k)} \quad \text{Eq.4.2}$$

Written in a form suitable for entry to modelling software, this appears as:

$$V=Vmax*S/(S+k) \quad \text{Eq.4.3}$$

In this generalised form of the equation, the resource concentration is S , the maximum rate of the processes is V_{max} , the output rate is V , and the value of S that enables V to attain 50% of the value of V_{max} (the so-called **half-saturation constant**) is k . This equation for the rectangular hyperbola will crop up many times in this book, in different guises with different variable names; its form will likely become instantly recognisable to you.

For the instance at hand, the resource is Am , the maximum rate is described by the constant $umax_Phy$, the output rate is u_Phy , and we need a half-saturation constant, which we will term kAm_Phy . This equation, for placement in the model thus reads as:

$$u_Phy = umax_Phy * Am / (Am + kAm_Phy) \quad \text{Eq.4.4}$$

or in standard mathematical notation as:

$$u^{Phy} = u_{max}^{Phy} \cdot \frac{Am}{(Am + k_{Am}^{Phy})} \quad \text{Eq.4.5}$$

From the equation, given that you can only add variables with the same unit, kAm_Phy can be seen to have the same units as Am (i.e., $\mu\text{gN L}^{-1}$). A default plausible value for kAm_Phy equates to $1\mu\text{M}$ ammonium, so here (as the mole mass of N is 14 g) we set $kAm_Phy = 14\ \mu\text{gN L}^{-1}$.

Revisiting the curve we considered earlier (Fig. 4.1), we can now redraw it (Fig. 4.3). Here the input value of V_{max} (here $umax_Phy$) is $0.693\ \text{d}^{-1}$; at infinite resource (Am) this is the plateau value of u_Phy . The value of k (as kAm_Phy) used in Fig. 4.3 can be seen to equate to a value of Am of $14\ \mu\text{gN L}^{-1}$; this supports a value of u_Phy of nearly $0.35\ \text{d}^{-1}$, which is half the value of $umax_Phy$ ($0.693\ \text{d}^{-1}$).

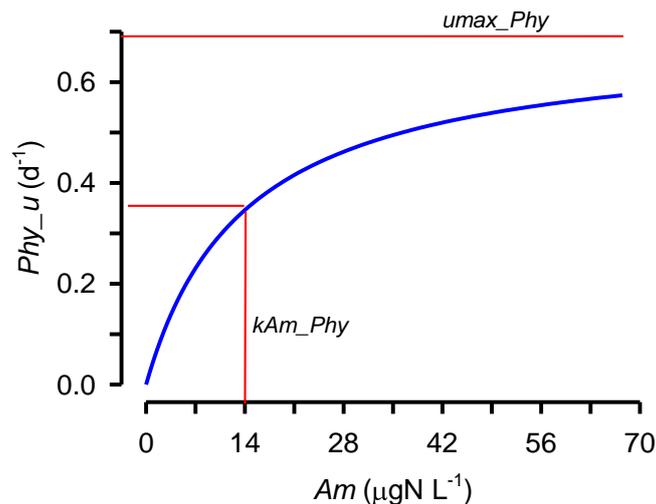


Fig. 4.3 Redrawn Fig. 4.1, with $umax_Phy = 0.693\ \text{d}^{-1}$, and kAm_Phy at a value of Am of $14\ \mu\text{gN L}^{-1}$.

NOTE: It is strongly recommended that response curves are always built and tested in a spreadsheet, driven by all plausible ranges of the stimulus or controller (x-axis) and plotted on x-y scatter graphs to see how the curve form describing the effector (output, y-axis) changes when the constants are altered. Only response curves that are well understood and accepted as appropriate for the task at hand should be transcribed into model code.

We now have all the model components in place, and we also have a defined set of connections between them to describe the relationship between ammonium concentration and phytoplankton growth making use to a response curve.

| Variable | Type | Value | Unit | Description |
|-----------------|------|--|-------------------------------------|--|
| <i>Am</i> | SV | 100 <i>-gro_Phy</i> | $\mu\text{gN L}^{-1}$ | Ammonium-N |
| <i>Phy</i> | SV | 1 <i>+gro_Phy</i> | $\mu\text{gN L}^{-1}$ | Phytoplankton biomass-N |
| <i>umax_Phy</i> | Con | 0.693 | $\text{gN gN}^{-1} \text{d}^{-1}$ | Phytoplankton maximum N-specific growth rate |
| <i>kAm_Phy</i> | Con | 14 | $\mu\text{gN L}^{-1}$ | Half saturation constant for <i>u_phy</i> |
| <i>u_Phy</i> | Aux | $\frac{umax_Phy * Am}{Am + kAm_Phy}$ | $\text{gN gN}^{-1} \text{d}^{-1}$ | Phytoplankton N-specific growth rate |
| <i>gro_Phy</i> | Aux | <i>u_Phy</i> * <i>Phy</i> | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Phytoplankton population growth rate |
| <i>sysN</i> | Aux | <i>Am</i> + <i>Phy</i> | $\mu\text{gN L}^{-1}$ | System N-balance |

Table 4.1 Simple N-limited phytoplankton model. See also Fig. 4.4. Variable types are state variables (SV), constants (Con), and auxiliary (Aux). The value for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

Note that the state variables have several pieces of information listed under “Value”. The first is the initial value; some thought needs to be considered here; clearly a value of 0 for initial nutrient concentration or initial phytoplankton biomass is going to yield something of a non-event. Logic is that, to drive a growth event, the initial value of *Am* is significantly greater than for *Phy* (initial values in the range of 100 and 1, respectively, would be good starting points here).

The other values indicate outputs (-) and inputs (+) into the state variables. The value of the flow (in this instance both defined by *gro_Phy*) are defined elsewhere in the equation set. You will have to describe the exits and entries to state variables according to the requirements of the modelling platform you use. When using a graphic-user-interface based platform, such as Powersim Studio, the act of linking the flow to the state variables (as in Fig. 4.4) automatically configures the differential equations.

4.8 Parameterising the Model

Papers and texts, reporting in detail different experimental methods for following phytoplankton growth in cultures, should be consulted if you intend to conduct real experiments to parameterise or validate your model. Here we consider the types of analyses, rather than the details. In all instances, as this is a dynamic simulation, you need to take samples frequently, ideally daily, if not twice a day.

- Obtain estimates for the input variables (“constants”) from the literature. Typical maximum growth rates for phytoplankton vary between ca. 2 divisions a day and $\frac{1}{4}$ division per day; these are specific growth rates of $2 \times 0.693 \text{ d}^{-1}$ and $0.25 \times 0.693 \text{ d}^{-1}$, respectively. You can readily measure cell-specific growth rates by following changes in cell abundance (using a microscope and haemocytometer) and applying Eq.4.1; at peak growth you can assume the cell-specific growth will be similar to N-specific growth (but see Section 4.11). Half-saturation constants for N-limited growth would be less than $1 \mu\text{M}$; accordingly expect a value of *kAm_Phy* of less than $14 \mu\text{gN L}^{-1}$. If you wish to describe P-limited growth instead, then the value will likely be much lower (ca. 10 fold lower); this reflects the higher affinity of

phosphate transport proteins in the phytoplankton cells. Note that the model as described requires half saturation values in units of mass L^{-1} , not as moles L^{-1} . Also note that these values are for half-saturation of growth, not of transport – see Flynn (1998) for discussion on this matter.

- Estimates of external nutrient concentrations require chemical analysis. If the unit for your model is N, then the easiest experiment to conduct would be using ammonium as the N-source; ammonium is more readily measured than is nitrate at the levels of sensitivity required. Ammonium can be measured spectrophotometrically, fluorometrically, or using an ammonium-specific electrode. At high concentrations in freshwater (but not in seawater), nitrate can be measured by nitrate-electrode rather than using a spectrophotometric approach. If using P, as phosphate, then a spectrophotometric method is typically used.
- Estimates of cellular nutrient (i.e., as described here, of phytoplankton-N) requires considerable significant effort and expense; it is usually determined by elemental analysis of samples captured onto ashed glass-fibre filters (phytoplankton-C is usually measured at the same time). An ashed filter is one that has been held at $500^{\circ}C$ for an extended period so that any organics are burnt off. Measurement of phytoplankton-P also requires cells to be collected onto an ashed filter, but the cells are then chemically oxidised so that cell-P is converted into phosphate and then measured in the same way as external (nutrient) phosphate is determined.
- The alternative to measuring cellular-nutrient is to make the assumption that all nutrient that was in the medium enters the organisms (which is indeed what the model assumes). Hence, the increase in phytoplankton-N, or phytoplankton-P, is obtained from the decrease in external nutrient concentrations.

4.9 Operating the Model

The model needs to be constructed within a platform capable of running an ordinary differential equation (ODE) -driven model. This matter is discussed in Chapter 2.7.

Before running the model, it is worth considering what types of output data should be plotted. Most obviously here, the state variables, together with the system balance ($sysN$ in Table 4.1) should be co-plotted (i.e., all upon one graph) against time.

In addition, it would be of interest to plot u_{Phy} against Am ; this is expected (of course) to return a plot of a rectangular hyperbola akin to that in Fig. 4.3.

Running the model for 20 days, with an integration step size of 1 day yields the outputs shown in Fig. 4.5.

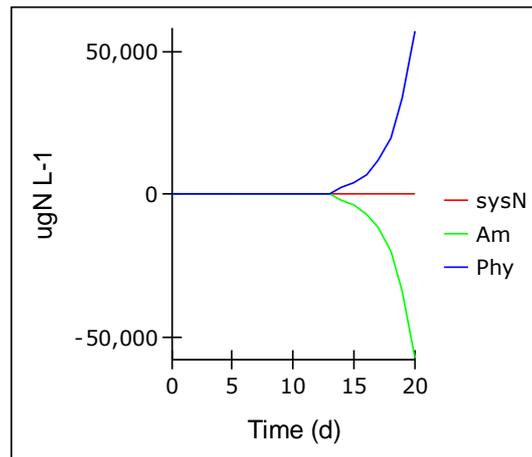


Fig. 4.5 Model output when the integration step size is far too large.

The most obvious point to note is that the state variable values are impossible, even though the system balance appears constant.

If the model is re-run advancing the simulation by one step at a time, the explanation for this output is readily observed; the transfer of *Am* to *Phy* becomes too great for the integration routine to correctly calculate it when operating with a time-step of 1 d.

Running the simulation again with the step size halved (0.5 d) and then halved again (0.25 d), and again (0.125 d), resolves the problem (Fig. 4.6).

Following a rule-of-thumb of using the step size half that of the value that gives acceptable results, a step size of 0.125 d is recommended for the model constructed as described in Table 4.1. There is now no unjustified oscillation in output values, and output values are sensible.

The plot of u_Phy against *Am* (Fig. 4.7) shows the expected rectangular hyperbolic relationship, with the values of maximum and half saturation constant overlain.

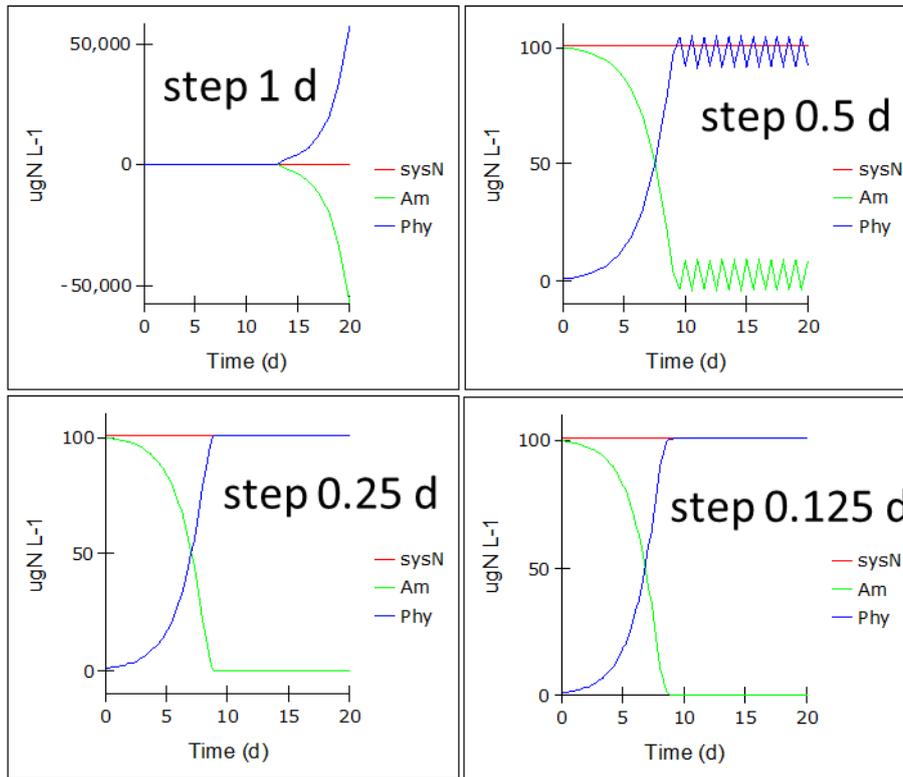


Fig. 4.6 Model operation with different integration step sizes. Note that for integration step sizes down to, and including, 0.25d, the concentration of Am goes negative beyond day 10, as shown by the values of the auto-scaling y-axis.

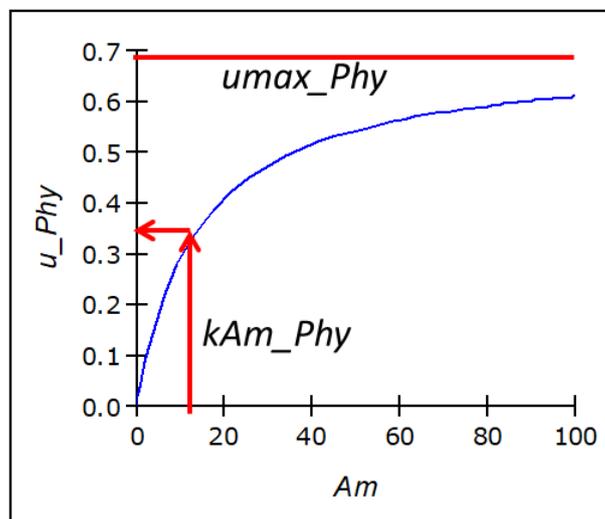


Fig. 4.7 Model output showing as a simulation output the underlying kinetics of nutrient limitation. Compare with Fig.4.3.

4.10 Things to Explore

- i) Try altering the values of the constants controlling the model, singularly and simultaneously, observing how the output changes.
- ii) Concurrently with (i) see what happens when you alter the integration step size, considering the values of the outputs and the real simulation time.
- iii) In competition, which is better, to have a high or low $umax_Phy$, and a high or a low kAm_Phy ?
- iv) Test your expectations from (iii) by modifying the model through introducing an additional state variable for another phytoplankton ($Phy2$) competing for the same resource Am , configured with constants $umax_Phy2$ and kAm_Phy2 . Alter $umax_Phy2$ and kAm_Phy2 , and see what happens during the competition.
- v) Revisit (iv) once you have installed the chemostat dilution components described in Chapter 7.
- vi) Add an additional auxiliary to enable a plot of cell numbers per L to be given. To do this requires a knowledge of the cell size, of the amount of C expected per cell volume, and the mass ratio of N:C within cells. Assume the following: the cells are spherical, with a diameter of $10\mu\text{m}$, and hence the volume can be computed by $4/3\pi r^3$; the cellular carbon density is 200gC L^{-1} (or more usefully here, given that a cubic μm is 1 fL, a density of 200 fgC fL^{-1}); assume a N:C mass ratio of 0.15. Note that this calculation makes various assumptions: the cultures is asynchronous (cells are at all different stages of the cell cycle); cell size does not vary with nutrient status (in reality it does; N-limited cells have a smaller diameter); N:C is constant (it is not; it will decline to more like 0.05 with N-starvation – see Chapter 15).
- vii) The model as described applies to biomass growth, assuming that growth conforms to a compound interest scenario. This would only equate simply to cell-specific growth if the cell divisions in the culture were randomly distributed over time. Real phytoplankton cells, growing in a light-dark cycle, tend to synchronise division to some portion of the dark phase. If you are considering cell division in a fully synchronised culture such that all cells suddenly divided, then the cell-specific growth rate would be zero until the instant of division. However, there is no instant in a model; the smallest unit of time is set by the `TIMESTEP`, so the division takes place over the duration of a timestep. The value of cell-specific growth rate aligning with a biomass-specific growth rate of $u=0.693\text{ d}^{-1}$, at that instant of cell division, is $1/\text{TIMESTEP}$, or more generally, $(u/0.693)/\text{TIMESTEP}$. **Note that this only works correctly using the Euler integration method.** Try producing a model for cell-specific growth that runs in parallel to the biomass-specific model you have built. You will need to consider the typical size of the cells (i.e., $\mu\text{gN cell}^{-1}$) and input the appropriate initial value into a new state variable describing $cells_Phy$ (cells L^{-1}) with reference to the initial value of Phy . Plot the changing value of $cell_N$ (i.e. $Phy/cells_Phy$). Because there is no direct link controlling the allocation of N to cells and their replication, gradually the simulated cell size will drift away from values you expect. In reality, that would not happen, as cells would only divide when they attain a given size. To complicate things further, that critical size for cell division changes with nutrient status and with temperature – see Flynn (2001) for a complex model describing such events.

4.11 Caveats

- Organism growth is more than just an increase in N biomass. For phytoplankton, exhaustion of the external nutrient (described here as N) does not result in an immediate cessation of growth. In reality the C-biomass and the cell number will increase for some time (possibly days) after exhaustion of the external nutrient. In this context the plot of growth is misleading, though it is actually correct when one considers N-specific growth. See Chapter 15.
- The model takes no account of any other nutrient. Although these are assumed to be non-limiting, in reality one of them will most likely become limiting; that “nutrient” is light. Unless the model is simulating a very low biomass system (very low Am), and growing in a small culture vessel, light will inevitably become limiting. This happens because as the culture grows it becomes increasingly pigmented and all that pigment shades light to the individual cells. In consequence the growth kinetics will not look as they do here, as an exponential curve which plateaus; instead, growth is expected to be more linear. See Chapter 8.
- The model assumes that all nutrients are accounted for. In reality, in an experiment, this is very rare. Phytoplankton cells may adhere to the culture vessel, thus removing them from the suspension, and they may also leak organic-N (notably as amino acids) which are not measured. Such events also create problems in parameterisation for it is very difficult to determine biomass lost by adherence to culture vessel walls, and far from trivial to measure forms of dissolved organic nutrients.
- It is worth considering that for a phototroph growing in a 12:12h light:dark cycle, net photosynthesis will have to occur at a rate more than twice 0.693 d^{-1} during the light phase, with a negative C-specific growth rate occurring at night due to the loss of C as CO_2 with respiration. Many phytoplankton divide at night (Nelson & Brand, 1979), so we must expect a clear asynchrony between cell-specific and C-specific growth rates. The assimilation of N over the light-dark cycle depends in part on the N-source and on the N-status of the phytoplankton (Clark et al. 2002). The lower the N-status (more N-starved) are the cells the more important is N-assimilation in darkness; cells growing with sufficient ammonium as the N-source primarily only assimilate the inorganic N concurrently with photosynthesis in the light.

4.12 Where Next

- In Chapter 6 we consider the traditional alternative to the description developed here; that is the Logistic equation. In that chapter the advantages of deploying a systems dynamic approach will become apparent.
- The subject of light limitation, of the development of self-shading, is explored further in Chapter 8. This will greatly enhance the models description of phytoplankton growth.
- Models that simultaneously describe C and N and also how pigment (chlorophyll) content varies with nutrient status have scope to give a much improved description of growth dynamics, with a decoupling of growth from external nutrient availability such that C-biomass increase continues after nutrient exhaustion. See Chapter 15.

5. A Simple Predator-Prey Model

Terms and concepts introduced in this chapter- rationalising simplifications, stoichiometry, ecological stoichiometry, regeneration, specific dynamic action

5.1 Ecological Context

The simplest, and most enduring, of biological models involve predator-prey interactions. We will come to the classic model, which describe the interactions in crude terms, in Chapter 6. Here we develop something which is actually significantly more realistic, which shows the flows of nutrients around the ecosystem. Such flows, the accounting of material between components of a system, are fundamental features defining the dynamics of ecology and the system dynamics approach. To build this model we will extend the description of the phytoplankton model built in Chapter 4 to include a predator to feed upon the phytoplankton prey, with the consequential nutrient recycling.

5.2 The Conceptual Model

The conceptual model sees the introduction of a predator (zooplankton) to eat the phytoplankton. In consequence of eating their prey, the zooplankton will release waste N that will recycle around the system. The conceptual model appears as Fig. 5.1. This shows a N-cycle between an inorganic nitrogenous resource (*Am*), a primary producer (*Phy*) and a secondary producer (*Zoo*). The system is closed; no N enters or leaves the system so $Am+Phy+Zoo$ is constant.

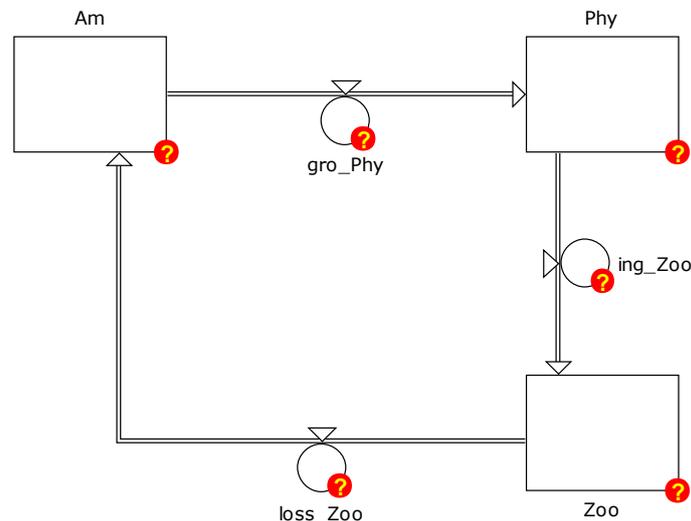


Fig. 5.1 Initial conceptual model. This is a Powersim Studio Forrester diagram representation. The “?” indicates that equations defining these variables have not been configured yet.

The ingestion of phytoplankton by the zooplankton population is termed *ing_Zoo* and the loss of N is *loss_Zoo*. It is worth noting that there is no immediately obvious analogue for the variable

gro_Phy in our previous model (see Fig. 4.4) that defines the growth of the zooplankton population. Instead, the growth of *Zoo* is given here as an emergent property of *ing_Zoo* minus *loss_Zoo*.

The flow labelled in Fig. 5.1 as *loss_Zoo* is comprised in reality of two distinct biological processes.

- i. Firstly there is the loss of ammonium that accompanies the release of CO₂ during respiration; this release is termed regeneration. Regeneration occurs because biological material has a ratio of elemental C:N that is constrained within certain limits; if C is lost then some N must be removed as well else the C:N deviates from biochemically acceptable bounds. Such a process is common to all consumers; humans release excess N in their urine and, for a given intake of water, the more protein-rich the diet, the darker (more concentrated) is that urine. Regeneration is associated with both the respiration associated with basic biological homeostasis and also the respiration associated with building new biomass, of which more detail is given below.
- ii. To the respiration-linked regeneration of N we add a second event, and that is the voiding as faeces of partly digested remnants of the food that is not assimilated. This is also an event common to all consumers, although for bacteria (which cannot ingest or egest particulate material) the unwanted material remains outside of the cell.

So, more correctly the model shown in Fig. 5.1 should look like Fig. 5.2.

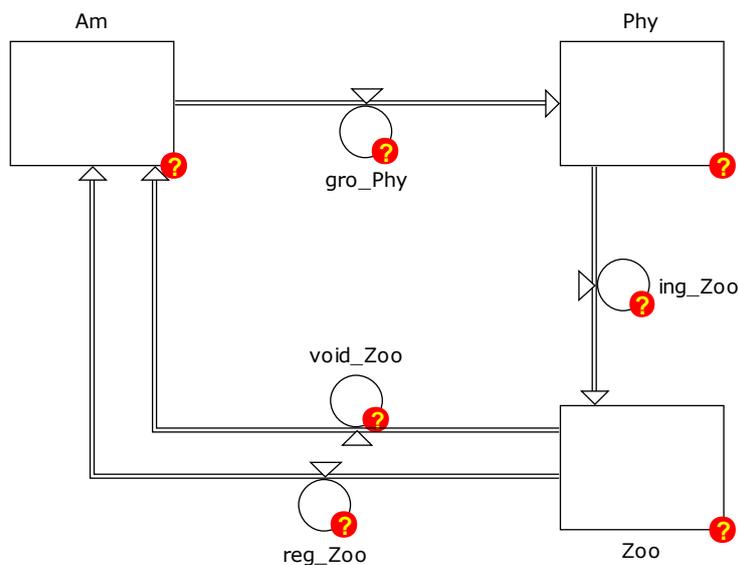


Fig. 5.2 Revised conceptual model, with inclusion of the loss terms from *Zoo*, labelled as *reg_Zoo* for regenerated N, plus *void_Zoo* accounting for the voiding of faecal material. This model assumes an instantaneous conversion of voided organic material back into inorganic nutrient (*Am*).

There is an assumption made in this model that both regenerated N and voided N (faeces and other organics) are converted instantaneously into ammonium. We turn now to justifying that simplification.

5.3 Rationalising the Simplifications

Rate *void_Zoo* describes the loss of voided material. In reality this material (which will be part dissolved and part particulate, depending on the level of digestion applied prior to voiding) will be degraded by bacteria. In addition, it could perhaps be used by the phytoplankton through mixotrophy via phagocytosis of particles and/or via osmotrophic activity; osmotrophy refers to the use of dissolved organics to support growth. Faecal material may also be reprocessed (eaten) by (most likely) zooplankton that lack sufficient of their preferred food.

To simplify things, just now let us assume that the N in the voided material is degraded to ammonium (state variable *Am* in the model) through processes that we will not detail here, and we assume that this process will be relatively fast. Check Section 2.3 “Flows” for a commentary on using “delay” functions.

The above represents a typical step in modelling, that of rationalising when and where to stop the description. During the construction, testing, and deployment of a model it is always worth revisiting such simplifying arguments, asking whether they are really justified and what implications are made both explicitly and implicitly. This is especially important when using a model under different scenarios, for which the original construction was not intended. An interesting example will be explore in Chapter 11, where we will consider how to include the activity of organisms beyond those we describe using state variables.

5.4 Configuring the Predator

We will proceed with configuring the revised model.

Ingestion

We may expect that the kinetics of zooplankton feeding upon its prey will be broadly similar to that we used for the phytoplankton consuming ammonium; that is, we may expect a type II response curve linking prey abundance to ingestion rate that saturates at high prey abundance. Accordingly we could consider deploying a rectangular hyperbola (see Fig. 4.1). In considering predation kinetics this curve is often incorrectly termed a “Holling type II” response curve; Holling type II (Holling 1965) actually describes an initial linear relationship with prey encounter and then a saturating phase associated with limitation at prey handling.

There are various reasons why the response curve relating abundance to resource acquisition would not be the same between dissolved nutrients and particulate food. Most obviously molecules do move in the same way as do particles (prey may well be motile, while molecules diffuse through the medium, affected by Brownian motion).

If you wish to research this more, then see Flynn & Mitra (2016) and Chapter 17. However, just for now we shall use a rectangular hyperbola of the same form that we used to describe ammonium uptake into phytoplankton in Chapter 4. We can thus set the half saturation for ingestion as a constant to be called *kPhy_Zoo*, working against the resource which is (of course) the concentration of prey, *Phy*. The maximum rate is defined by *ingmaxPhy_Zoo*, so the N-specific ingestion rate, *ingPhy_Zoo* (with units of $\text{gN gN}^{-1} \text{d}^{-1}$), is described as:

$$ingPhy_Zoo = ingmaxPhy_Zoo * Phy / (Phy + kPhy_Zoo) \quad \text{Eq.5.1}$$

To prevent extinction of the prey, we can include a threshold value below which predation does not occur. In essence, below this threshold abundance level the prey are *de facto* invisible. Including this threshold (*thresPhy*), the description becomes:

$$ingPhy_Zoo = ingmaxPhy_Zoo * (Phy - thresPhy) / (Phy - thresPhy + kPhy_Zoo) \quad \text{Eq.5.2}$$

The form of the equation is perhaps more clearly written thus:

$$ing_{Phy}^{Zoo} = ingmax_{Phy}^{Zoo} \cdot \frac{(Phy - thres_{Phy})}{((Phy - thres_{Phy}) + k_{Phy}^{Zoo})} \quad \text{Eq.5.3}$$

From this you can more readily appreciate that the variable describing the substrate within the rectangular hyperbola equation (Cf. Eq.4.2) is now defined as (*Phy-thres_{Phy}*).

Of course this equation is only valid when it returns a positive value, when *Phy* >= *thresPhy*. To prevent an error being generated we could introduce a conditional term; the syntax of this will vary depending on the modelling platform that you are using. For example, the description of ingestion could be written as:

$$ingPhy_Zoo = IF(Phy > thresPhy, ingPhy_{max}_Zoo * (Phy - thresPhy) / (Phy - thresPhy + kPhy_Zoo), 0) \quad \text{Eq.5.4}$$

This syntax reads “IF ({condition is true},{do this}, {otherwise do this})”.

The value of the population ingestion rate (the total consumption of the prey, *Phy*), *ing_Zoo* (gN L⁻¹ d⁻¹), is thus:

$$ing_Zoo = ingPhy_Zoo * Zoo \quad \text{Eq.5.5}$$

Voiding and assimilation

No consumer assimilates everything that it eats. Indeed, the more food that is available the more wasteful is a consumer in this regard; why expend effort to digest every last part of a meal if a more digestible option is available?

The proportion that is assimilated may be defined by reference to an assimilation efficiency, *AE*. In reality, the value of *AE* will not only vary with the quantity of food, it will vary with the quality of the food. Thus *AE* for carbon, which we can term *AE_C* and defines the proportion of ingested food-C that actually crosses the gut or feeding vacuole membranes into the consumer cells, will invariably be different to that for nitrogen, *AE_N*. It may thus be readily appreciated that the C:N ratio of different food options will affect the potential value of the food for nutrition of the consumer. Further, the difference in the C:N of the food relative to the C:N of the consumer will also affect the value of assimilation efficiency.

The ratio of one chemical to another is termed its **stoichiometric ratio**. In this instance the ratio is of C:N. The subject of stoichiometry is of great importance in trophic dynamics, and thence the dynamics of ecology, because where there is an imbalance of supply and demand, the excess must be removed.

A whole branch of ecology has been developed around this topic of **ecological stoichiometry** (Sterner & Elser 2002). The strongest interactions typically involve primary producers (here, phytoplankton) because usually they have a C:N ratio higher than that of the consumer (here,

zooplankton). There is thus too much C in the food relative to N, so less C will (can) be assimilated; $AE_C < AE_N$. We do not need to worry about these complexities just now, because our simple model uses N as the sole currency. Likely, however, the potential for interesting implications of variable C:N will not be lost on the reader; we will revisit this topic in Chapters 15, 16 & 17.

For simplicity, and because our model describes N as the sole element, we will declare a constant value for AE, and to remind ourselves that it is for N, we will term it AEN_{Zoo} . The value of AEN_{Zoo} has no units; it is a proportion.

The amount of ingested food assimilated by the zooplankton, $assN_{Zoo}$ ($N N^{-1} d^{-1}$), is thus given as:

$$assN_{Zoo} = ingPhy_{Zoo} * AEN_{Zoo} \quad \text{Eq.5.6}$$

The amount that is voided is the balance of ingestion minus assimilated; as the proportion assimilated is given by AE, then the proportion that is voided will be (1-AE). We thus define the value of zoo_void ($gN L^{-1} d^{-1}$) as:

$$void_{Zoo} = ing_{Zoo} *(1- AEN_{Zoo}) \quad \text{Eq.5.7}$$

Or we could define it more completely (showing the origins of the event) as:

$$void_{Zoo} = ingPhy_{Zoo} * Zoo *(1-AE_N) \quad \text{Eq.5.8}$$

Respiration & regeneration

Another consequence of stoichiometry is that as organisms respire (produce CO_2 and hence lose biomass-C) then they must also lose other elements. If this did not occur (and it happens as a consequence of the underlying biochemistry) then the organism C:N would fall to values that would be impossible. For example, you could not have an organismal C:N of 1; the minimum C:N mass ratio is around ca. 4. Here we are concerned with N, and hence as respiration occurs biomass-N is lost; we assume here that this is lost as ammonium-N and directly re-enters the Am state variable.

As mentioned earlier, there are two main types of respiration that we can identify. These are associated with catabolism (generating energy to enable the organism to maintain homeostasis and functionality, motility, etc.), and that associated with anabolism (making new proteins, biomass, etc.).

The catabolic respiration, which we will term **basal respiration**, occurs all the time, irrespective of whether food is being assimilated. In reality, we can well imagine that this value will vary, for example for a motile consumer while hunting, declining when satiated. For simplicity we can consider it as a constant. So, every day a proportion of zooplankton biomass (Zoo) is *de facto* “burnt off”, respired, with a commensurate regeneration of biomass-N as ammonium-N (Am). We will scale this respiration to the maximum growth rate of the zooplankton, using the constant BR_{Zoo} . The reason for this is to reflect the higher respiration rates in faster growing, and thus more active, organisms.

In addition, there is the cost of assimilating food into new biomass. This cost, sometimes called metabolic respiration, is related to a process termed in the literature as **specific dynamic action (SDA)**. What the value of SDA tells us is that, for example, per gram of ingested protein-N, how many grams of N will be lost during assimilation of the remainder into consumer biomass. This is in

addition to losses due to other metabolic activities and relates to functioning of biochemical pathways of catabolism and anabolism. The value of *SDA* differs depending on the nature of the food, whether it is primarily carbohydrate, protein, fats etc. Values of *SDA* for carbohydrates and fats are of the order of 5-15%, and for protein they are 20-35%.

Our model is N-based, and ca. 75% of a phytoplankton cell-N is protein, the remainder of the N being mainly in the nucleic acids DNA and RNA. Let us assign a constant *SDA* with a value of 0.3 (30%), and recall that this applies to the proportion of the material ingested that was actually assimilated (i.e., not voided).

The total specific N-regeneration rate, that is gN per g of zooplankton N-biomass per day (*regN_Zoo*; gN gN⁻¹ d⁻¹), is thus given as:

$$regN_Zoo = (umax_Zoo * BR_Zoo) + assN_Zoo * SDA \quad \text{Eq.5.9}$$

The total regenerated by the zooplankton population (*zoo_regen*; gN L⁻¹ d⁻¹) is:

$$zoo_regen = regN_Zoo * Zoo \quad \text{Eq.5.10}$$

5.5 Establishing the Zooplankton Maximum Ingestion Rate

Often the growth rate of the zooplankton is described as an emergent property of ingestion minus loss processes. Following this argument, the maximum possible growth rate is thus controlled by the input value (constant) defining the maximum possible ingestion rate. Accordingly, the consumer would have to eat all the time at the maximum rate in order to attain its maximum growth rate. This is not how real consumers work.

In real consumers, the maximum rate of ingestion is many times faster than required to sustain maximum growth; a complex series of feedback processes then modulates feeding as a function of satiation. We do not need to go to that level of complexity here, but we can readily configure the model so that at least the maximum possible growth rate controls the dynamics, rather than the maximum feeding rate being in control. To achieve this we need to define the maximum ingestion rate as a function of the maximum growth rate and the allied cumulative values of the loss rates.

In words, we have:

$$\{growth\ rate\} = \{ingestion\} - \{voiding\} - \{anabolic\ regeneration\} - \{catabolic\ regeneration\} \quad \text{Eq.5.11}$$

In full this appears like this:

$$u^{Zoo} = ing_{Phy}^{Zoo} - \left(ing_{Phy}^{Zoo} \cdot (1 - AE_N^{Zoo}) \right) - \left(ing_{Phy}^{Zoo} \cdot AE_N^{Zoo} \cdot SDA \right) - (u_{max}^{Zoo} \cdot BR^{Zoo})$$

This simplifies to:

$$u^{Zoo} = ing_{Phy}^{Zoo} \cdot \left((1 - (1 - AE_N^{Zoo})) - (AE_N^{Zoo} \cdot SDA) \right) - (u_{max}^{Zoo} \cdot BR^{Zoo})$$

$$u^{Zoo} = ing_{Phy}^{Zoo} \cdot AE_N^{Zoo} \cdot (1 - SDA) - (u_{max}^{Zoo} \cdot BR^{Zoo}) \quad \text{Eq.5.12}$$

Rearranging and, assuming non-limiting prey, replacing ing_{Phy}^{Zoo} with the maximum ingestion rate (ing_{maxPhy}^{Zoo}) and u^{Zoo} with the maximum growth rate (u_{max}^{Zoo}) we obtain, in a form ready for the model code, the definition of ing_{maxPhy}^{Zoo} as:

$$ingmaxPhy_Zoo = (umax_Zoo*(1+BR_Zoo))/(AEN_Zoo*(1-SDA)) \tag{Eq.5.13}$$

By setting $ingmaxPhy_Zoo$ in this fashion, we can now define the maximum growth rate, and the modelled zooplankton will do as a real consumer will, and modify ingestion according to how “hungry” it is. So, if we subjected the zooplankton to stress, so that AE decreased and BR increased, then if there was sufficient food available the zooplankton could still grow at its maximum rate by eating more. If we configured the model with the maximum ingestion rate as a constant, our modelled zooplankton could not modify its behaviour to counter stress in this fashion.

5.6 The Model

We now have all components for the new model. The model schematic is given in Fig. 5.3, and the full set of equations, including the phytoplankton components reproduced from the previous chapter, are given in Table 5.1.

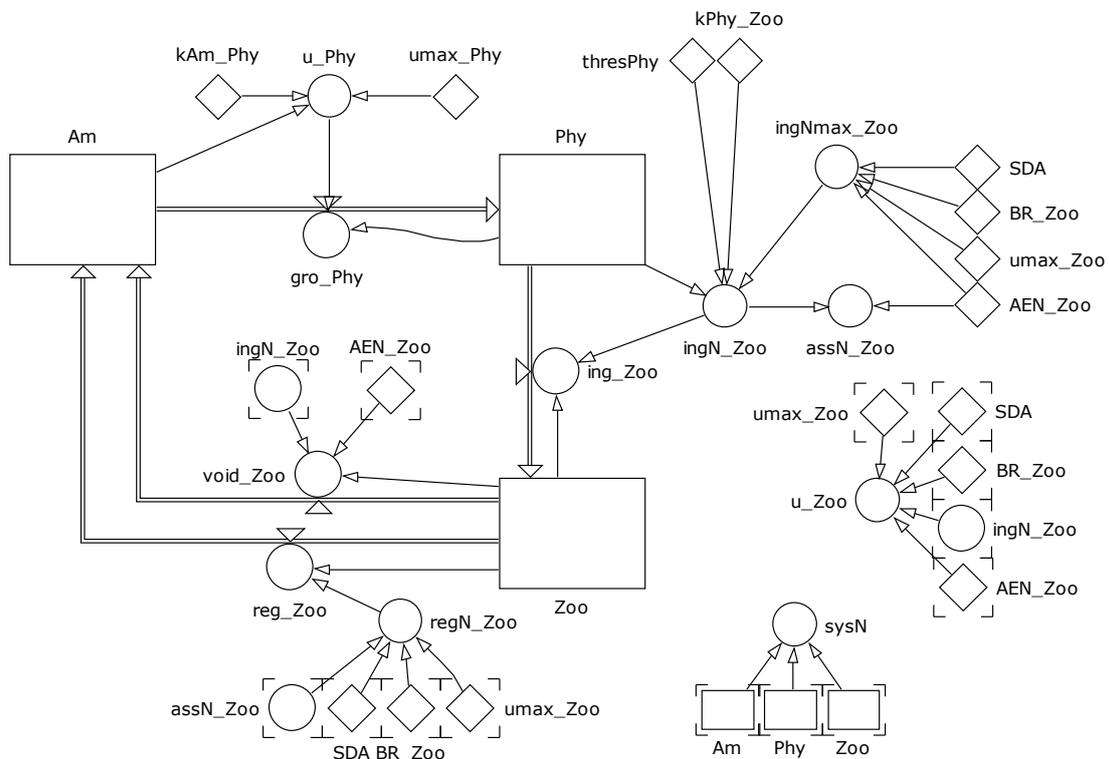


Fig. 5.3 The complete model as per Table 5.1. See legend for Fig. 2.2 for an explanation on the format of the Forrester diagram.

| Variable | Type | Value | Unit | Description |
|--------------------|------|---|--------------------------------------|--|
| <i>Am</i> | SV | 100 <i>- gro_Phy</i> <i>+ reg_Zoo</i> <i>+ void_Zoo</i> | µg N L ⁻¹ | Ammonium-N |
| <i>Phy</i> | SV | 1 <i>+ gro_Phy</i> <i>- ing_Zoo</i> | µg N L ⁻¹ | Phytoplankton N-biomass, changing with growth and losses to ingestion into zooplankton |
| <i>Zoo</i> | SV | 0.1 <i>+ ing_Zoo</i> <i>- reg_Zoo</i> <i>- void_Zoo</i> | µg N L ⁻¹ | Zooplankton N-biomass, changing with ingestion of phytoplankton and losses to regeneration and voiding |
| <i>AEN_Zoo</i> | Con | 0.6 | dl | Assimilation efficiency for N |
| <i>BR_Zoo</i> | Con | 0.1 | dl | Index of basal (catabolic) respiration |
| <i>kAm_Phy</i> | Con | 14 | µg N L ⁻¹ | Half saturation constant for <i>u_Phy</i> |
| <i>kPhy_Zoo</i> | Con | 42 | µg N L ⁻¹ | Half saturation constant for <i>ingN_Zoo</i> |
| <i>SDA</i> | Con | 0.3 | gN gN ⁻¹ | Specific dynamic action (anabolic respiration cost for assimilating N) |
| <i>thresPhy</i> | Con | 0.014 | µg N L ⁻¹ | Threshold for predation |
| <i>umax_Phy</i> | Con | 0.693 | gN gN ⁻¹ d ⁻¹ | Maximum specific growth rate of the phytoplankton |
| <i>umax_Zoo</i> | Con | 1.5 | gN gN ⁻¹ d ⁻¹ | Maximum specific growth rate of the zooplankton |
| <i>assN_Zoo</i> | Aux | <i>ingN_Zoo</i> * <i>AEN_Zoo</i> | gN gN ⁻¹ d ⁻¹ | Assimilation rate |
| <i>gro_Phy</i> | Aux | <i>Phy</i> * <i>u_Phy</i> | µg N L ⁻¹ d ⁻¹ | Phytoplankton population growth rate |
| <i>ing_Zoo</i> | Aux | <i>Zoo</i> * <i>ingN_Zoo</i> | µg N L ⁻¹ d ⁻¹ | Zooplankton population ingestion rate |
| <i>ingN_Zoo</i> | Aux | $IF(Phy > thresPhy, ingNmax_Zoo * (Phy - thresPhy) / (Phy - thresPhy + kPhy_Zoo), 0)$ | gN gN ⁻¹ d ⁻¹ | Ingestion rate with inclusion of threshold control |
| <i>ingNmax_Zoo</i> | Aux | $(umax_Zoo * (1 + BR_Zoo)) / (AEN_Zoo * (1 - SDA))$ | gN gN ⁻¹ d ⁻¹ | Maximum ingestion rate |
| <i>reg_Zoo</i> | Aux | <i>Zoo</i> * <i>regN_Zoo</i> | µg N L ⁻¹ d ⁻¹ | Zooplankton population N-regeneration rate |
| <i>regN_Zoo</i> | Aux | $(umax_Zoo * BR_Zoo) + assN_Zoo * SDA$ | gN gN ⁻¹ d ⁻¹ | Zooplankton N-specific regeneration rate |
| <i>sysN</i> | Aux | <i>Am</i> + <i>Phy</i> + <i>Zoo</i> | µg N L ⁻¹ | System N-balance |
| <i>u_Phy</i> | Aux | $umax_Phy * Am / (Am + kAm_Phy)$ | gN gN ⁻¹ d ⁻¹ | Phytoplankton N-specific growth rate |
| <i>u_Zoo</i> | Aux | $ingN_Zoo * AEN_Zoo * (1 - SDA) - (umax_Zoo * BR_Zoo)$ | gN gN ⁻¹ d ⁻¹ | Zooplankton N-specific growth rate |
| <i>voidN_Zoo</i> | Aux | <i>Zoo</i> * <i>ingN_Zoo</i> *(1- <i>AEN_Zoo</i>) | µg N L ⁻¹ d ⁻¹ | Zooplankton population N-voiding rate |

Table 5.1 Simple N-limited phytoplankton-zooplankton model. See Fig. 5.3. dl - dimensionless. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

5.7 Parameterising the Model

Papers and texts reporting in detail experimental methods should be consulted if you intend to conduct real experiments to obtain data to parameterise or validate your model. Here we consider the types of analyses, rather than the details. In all instances, as this is a dynamic simulation, you need to take samples frequently, ideally daily, if not twice a day.

- Obtain estimates for the constants from the literature for the species you are considering. For the prey, see Section 4.8. For the predator see also Flynn & Mitra (2016).
- External nutrient is measured as described in Section 4.8.
- Total (i.e., prey+predator) particulate-N is measured as described in Section 4.8. Faecal material (which is likely to also include bacterial biomass) can become significant; this will be included within this fraction of prey+predator, assuming the particles are large enough to be trapped on the filters. Micro-faecal material, and also forms of dissolved organic-N may accumulate (see e.g., Flynn & Davidson 1993) and may not be measured readily.
- Determination of biomass for the individual organism types (prey or predator) is extremely challenging in such systems as it is often very difficult (if possible at all) to separate the organisms. As alternatives, organism counts can be taken to at least assign relative rates of increase and decrease of the populations. However, as this is a N-based model an assumption must be made that the N-content remains constant per organism (which is most unlikely) and aligns in a fixed stoichiometric proportion to the C-content (see Menden-Deuer & Lessard 2000).

5.8 Operating the Model

Fig. 5.4 gives some example output run using the input values in Table 5.1, operating with an integration step size of 0.0625 d^{-1} under an Euler integration scheme.

There are some immediate observations to make. Firstly, the system dynamics oscillate, and by adjusting the parameter values (see Section 5.9) these oscillations can be dampened or strengthened. Secondly, note from the x-y scatter plots that the relationship between consumer abundance and resource abundance is anything but simple. These plots display an attractor basin (see Section 2.11 “Data visualisation”) for the interaction. This demonstrates one of the important reasons for operating systems dynamics models – through such approaches we can better understand why it is so difficult, perhaps even dangerous, to attempt to make correlations between features of ecology such as abundances and rate processes using data taken at one or just a few random selected points in time and space. Cause-and-effect is difficult to resolve in real dynamic systems and simulations provide a platform for exploring why.

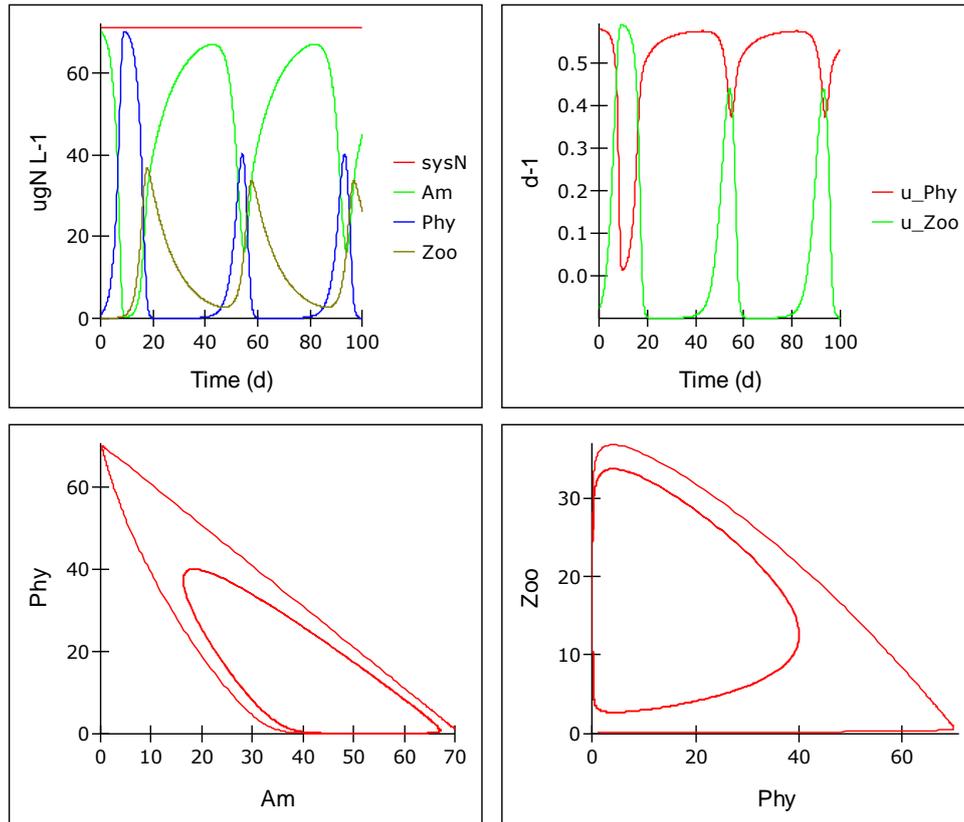


Fig. 5.4 Example model output, with initial values for *Am*, *Phy* and *Z* at 70, 1, 0.1 $\mu\text{gN L}^{-1}$ respectively. Note that 14 $\mu\text{gN L}^{-1}$ equates to 1 $\mu\text{M N}$. Note the lower panels show the dynamics of the system tending towards attractor basins (see Section 2.11, Data visualisation).

5.9 Things to Explore

- i) Try altering the values of the constants in the phytoplankton description singularly and also together, observing how the output changes.
- ii) Try altering the values of the constants for the zooplankton description singularly and also together, observing how the output changes. Which constants have the biggest impact for the rate of consumption of the phytoplankton population (*Phy*) and the development of zooplankton biomass (*Zoo*)?
- iii) Concurrently with (i) and (ii) see what happens when you alter the integration step size. What you should notice is that if the dynamics are more abrupt then the step size needs to be smaller. Always check your model output for such situations.
- iv) How does altering the value of the initial *Am* concentration, and values of *thresPhy* and *kPhy_Zoo* affect the development of cycles in trophic dynamics? In particular try very low values of *thres* (including 0).
- v) How does altering the relative values of *umax_Phy* and *umax_Zoo* affect the development of cycles in trophic dynamics?

- vi) Think of factors that may affect the selective advantage for different configurations of phytoplankton. Are these all reflected in the current model structure? Compare your views now with the responses you made from Section 4.10, part (iv).
- vii) Revisit the above once you have installed the chemostat dilution components described in Chapter 7.
- viii) Consider delaying the regeneration of Am from voided material from Zoo . If your software permits, you can do this easily using a pipeline delay routine (see Section 2.3 “Flows”).

5.10 Caveats

- The same caveats as applied to the phytoplankton-only components (Section 4.11) apply here, but the situation is complicated greatly by the presence of the predator and in reality by the presence of faecal material.
- The accumulation of faecal material, which is not explicitly simulated here, may be significant. It may be reprocessed by the predator when the phytoplankton prey abundance falls (Flynn & Davidson 1993), and/or bacterial degradation may occur that regenerates the N in a form suitable for use by the phytoplankton far more slowly than the instantaneous regeneration considered here.

5.11 Where Next

- In Chapter 6 we consider the traditional alternative to the description developed here; that is the Lotka-Volterra approach. In that chapter the advantages of deploying a systems dynamic approach will become apparent.
- Light limitation of the growth of the prey is an important factor impacting on the total dynamic; we consider this further in Chapter 8 and 10.
- Predation, or feeding, does not really operate in a fashion that is best described by a rectangular hyperbola. On the contrary, such a description can give an output that cannot conform to reality (Flynn & Mitra 2016; Chapter 17).

6. Logistic and Lotka-Volterra Models

Terms and concepts introduced in this chapter- Logistic equation, carrying capacity, Lotka-Volterra, matching and mismatching, empirical vs mechanistic, dysfunctionality

6.1 Ecological Context - a Historic Diversion

A feature common in all real biological systems is the non-linear density dependence of rate processes. In other words, as the abundance of resources and of biomass of different organisms changes so the rates of growth and so on do not change *pro rata*, in a simple fashion. So far we have considered such dynamics using an explicit link to resource availability (as nutrient or food) through the use of rectangular hyperbolic functions (Chapters 4 & 5). However, this is not how density-dependence has been described in models in classic theoretical ecology.

Classically, and with an eye to the pragmatic reality of lacking conceptual and numeric information to do otherwise, such relationships have been described using wholly empirical approaches that simply describe the fact that growth does not continue for ever (something must restrict it, but we do not know what) and that predator-prey interactions also involve process that display cyclic density dependence (again, relating to some factors about which we are not quite sure). These classic descriptions are the **Logistic equation** and **Lotka-Volterra** (L-V) models.

Traditionally, a text on dynamic ecology would have started with these two models. Scientists now have a much firmer grasp of how real systems work, and our computational abilities are also much improved, such that we can now explicitly involve controlling factors that we were formally ignorant of and/or could not readily model. It is nonetheless useful to see how these tradition approaches operate in comparison with systems dynamic approaches.

6.2 The Logistic Equation Model

The logistic equation has a long history in economics and ecology (for extensive details and discussions, Google “Verhulst”, “Malthus” and “logistic equations”). The equation describes the growth, and thence the final size of a population, as a function of its growth rate “ r ” and what is termed the system **carrying capacity**, “ K ”. (Do not confuse this K with the half saturation constant in the rectangular hyperbolic Michaelis-Menten and Monod equations.)

The increase in population size is related to its current size (Pop) and its growth rate r (i.e., growth = $Pop * r$). The decrease in population size (die back) is described in logistic equations according to a power function of the population size, such as $r * Pop^2/K$; we will revisit this part in the guise of a “closure function” in Chapter 11.

A Forrester diagram representation of the Logistic Equation model is given in Fig. 6.1, with the equations in Table 6.1.

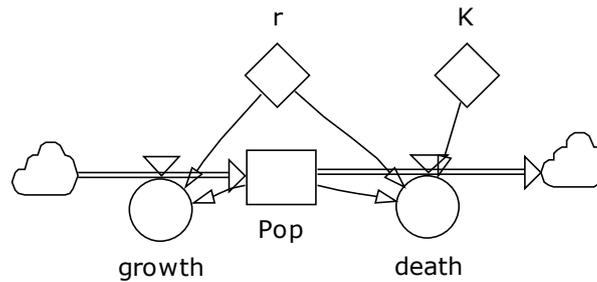


Fig. 6.1 Logistic model structure. The clouds represent entry and exit flows that are not explicitly described in the model formulation.

| Parameter | Type | Value | Unit | Description |
|---------------|------|--------------------------|---------------------------------------|---|
| <i>Pop</i> | SV | 1 + growth - death | nos | Population size |
| <i>K</i> | Con | 100 | nos | Carrying capacity (maximum <i>Pop</i>) |
| <i>r</i> | Con | 0.693 | nos nos ⁻¹ d ⁻¹ | Populations-specific growth rate |
| <i>death</i> | Aux | $r \cdot Pop^2 / K$ | nos d ⁻¹ | Death rate |
| <i>growth</i> | Aux | $r \cdot Pop$ | nos d ⁻¹ | Growth rate |

Table 6.1 Equations and parameters for a Logistic model. See Fig. 6.1. The value for the state variable is for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

While we are here, it is worth noting how these equations are reported in standard mathematical formulae, and the relationship with the code above.

The rate of change in the population size would be reported typically as:

$$\frac{dPop}{dt} = r \cdot Pop \cdot \left(1 - \frac{Pop}{K}\right) \tag{Eq.6.1}$$

Which after rearranging reads as:

$$\frac{dPop}{dt} = r \cdot Pop - \frac{r \cdot Pop^2}{K} \tag{Eq.6.2}$$

In Eq.6.2 the inflow and outflow, as entered into modelling code (Table 6.1), can be readily identified.

Some example output is shown in Fig.6.2.

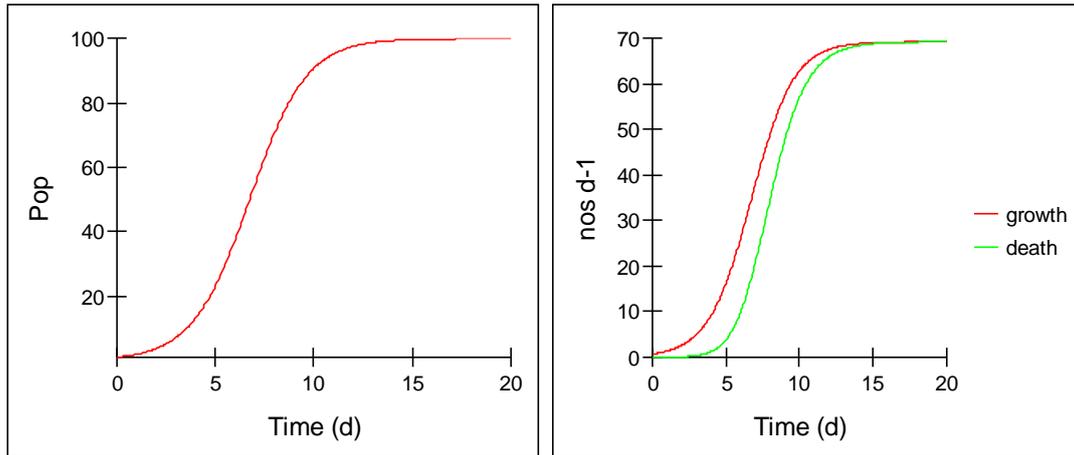


Fig. 6.2 Example Logistic model output. The left panel shows the population density, while the right panel shows the growth and death rates; when these are balanced (from ca. time 15 onwards) the population density stabilises.

6.3 Things to Explore with the Logistic Equations

- i) What happens when you change “ r ”?
- ii) What factors could change “ r ” in an ecological or physiological context?
- iii) What happens when you change “ K ”?
- iv) What factors could change “ K ” in an ecological context?
- v) How helpful is the model, in general, and as applied in reality?

6.4 Logistic Equation vs Systems Ecology

The most obvious difference between the construction and behaviour of the Logistic Equation for growth, in comparison with the systems ecology style phytoplankton growth model we built in Chapter 4, is that with the Logistic Equation there is no explicit linkage to resource availability. In fact, there is no stated resource in the Logistic model; while you could argue it is reflected by the value of K , in reality other factors such as over-crowding rather than resource could limit growth.

The decay in net growth rate in the Logistic model is all based around death, not growing more slowly, while in Chapter 4 the model did not consider death, but only resource-limited growth. Of course, with the phytoplankton model in Chapter 4 we could easily have introduced a function describing death, and link that to the population numeric density, and/or to population health as reflected by the specific-rate of growth relative to the maximum potential rate of growth (i.e., health = μ/μ_{\max}). That would have given us an explicit, rather than implicit, description of the dynamics and hence could provide a better understanding of what is really happening.

6.5 The Lotka-Volterra (L-V) Model

In many ways L-V models can be considered as the progenitor of predator-prey models. The operation of L-V models describes apparently realistically looking cycles of prey and predator abundance, with degrees of matching or mismatching (i.e., alignment of prey and predator abundances) depending on the constants used.

Like the Logistic Equation, however, there is no attempt to secure a system balance, to account for the transfer of a specific amount of material between resource and consumer (here, prey and predator). So, as with the Logistic Equation there is no resource limitation; no resource is actually specified either for the prey or for the predator.

As in the Logistic Equation, Prey (*Prey*) grows exponentially (*gro_Prey*; $Prey\ d^{-1}$), governed by a specific rate constant $k1\ (d^{-1})$. This constant $k1$ is analogous to r in the Logistic equation as described above (Eq.6.1).

$$gro_Prey = k1 * Prey \quad \text{Eq.6.3}$$

The loss of *Prey* (*death_Prey*; $Prey\ d^{-1}$) is defined as a function of predator abundance (*Pred*) and of prey abundance (*Prey*) with constant $k2$. The units of $k2$ are $Pred^{-1}\ d^{-1}$; $k2$ thus states the number of prey removed per predator per day. While this rate of predation is a function of prey abundance (i.e., at the limit there is sort of a resource limitation) the function does not saturate at an upper limit, and the rate of loss of *Prey* is in part a function of the prey abundance itself.

$$death_Prey = k2 * Prey * Pred \quad \text{Eq.6.4}$$

Growth of the predator (*gro_Pred*; $Pred\ d^{-1}$) is related to the abundance of the prey population via constant $k3$ in an analogous fashion to the death of prey. Constant $k3$ has units of $Prey^{-1}\ d^{-1}$.

$$gro_Pred = k3 * Prey * Pred \quad \text{Eq.6.5}$$

Death of the predator (*death_Pred*; $Pred\ d^{-1}$) is a specific rate of its abundance, defined by $k4\ (d^{-1})$.

$$pred_death = k4 * Pred \quad \text{Eq.6.6}$$

As differential equations, the rate of change of *Prey* and *Pred* thus looks like this:

$$\frac{dPrey}{dt} = Prey \cdot (k1 - k2 \cdot Pred) \quad \text{Eq.6.7}$$

$$\frac{dPred}{dt} = -Pred \cdot (k4 - k3 \cdot Prey) \quad \text{Eq.6.8}$$

Rearranged, we obtain

$$\frac{dPrey}{dt} = k1 \cdot Prey - k2 \cdot Prey \cdot Pred \quad \text{Eq.6.9}$$

$$\frac{dPred}{dt} = k3 \cdot Prey \cdot Pred - k4 \cdot Pred \quad \text{Eq.6.10}$$

The model is shown in Fig. 6.3.

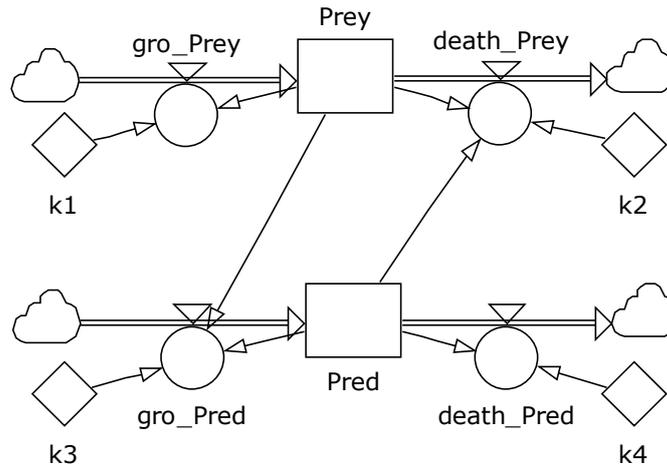


Fig. 6.3 L-V model structure. Note there is no explicit flow of material from prey to predator, just an implicit linkage. The clouds represent entry and exit flows that are not explicitly described in the model formulation. There is no indication of a linkage between predator activity and resource recycling back to *Prey* either, nor of a resource being used by *Prey* (Cf. Chapter 5)

| Parameter | Type | Value | Unit | Description |
|-------------------|------|--|---|--------------------------------------|
| <i>Pred</i> | SV | 10 <i>+ gro_Pred</i> <i>- death_Pred</i> | <i>Pred</i> nos | Predator population size |
| <i>Prey</i> | SV | 1 <i>+ gro_Pred</i> <i>- death_Pred</i> | <i>Prey</i> nos | Prey population size |
| <i>death_pred</i> | Aux | $k4 * Pred$ | <i>Pred</i> d ⁻¹ | Predator loss |
| <i>gro_pred</i> | Aux | $k3 * Pred * Prey$ | <i>Pred</i> d ⁻¹ | Predator gain |
| <i>death_prey</i> | Aux | $k2 * Pred * Prey$ | <i>Prey</i> d ⁻¹ | Prey loss |
| <i>gro_prey</i> | Aux | $k1 * Prey$ | <i>Prey</i> d ⁻¹ | Prey gain |
| <i>k1</i> | Con | 0.693 | d ⁻¹ | Prey-specific growth rate |
| <i>k2</i> | Con | 0.5 | <i>Pred</i> ⁻¹ d ⁻¹ | Predator-specific prey loss constant |
| <i>k3</i> | Con | 0.2 | <i>Prey</i> ⁻¹ d ⁻¹ | Prey-specific predator growth rate |
| <i>k4</i> | Con | 0.4 | d ⁻¹ | Predator-specific predator loss rate |

Table 6.2 L-V model equations. The value for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

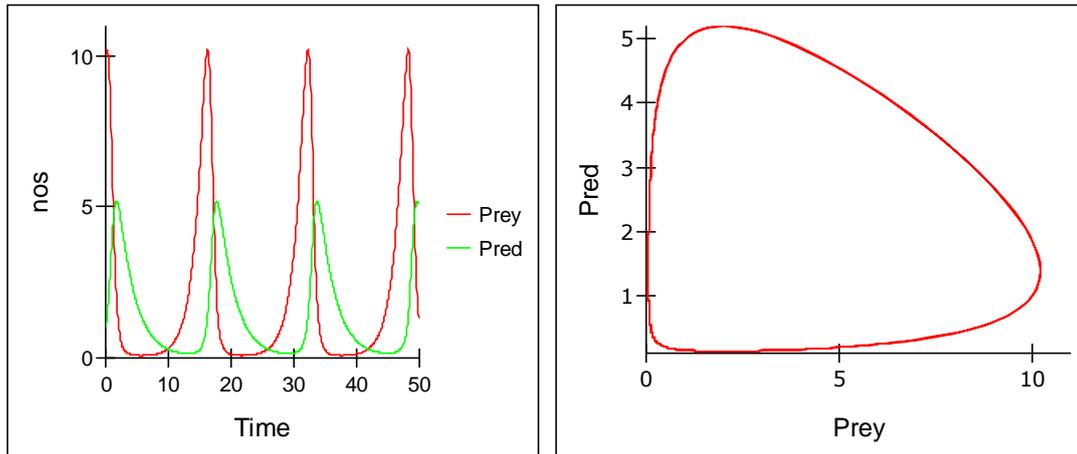


Fig. 6.4 Example L-V model output run using a R-K4 integration routine. If using Euler a very small step size is needed to recreate these dynamics because of the cumulative errors in running the Euler routine which are unconstrained in the L-V model. This is because there is no cycling of nutrients that would provide a control (constraint) of the non-linear processes that are involved in reality, and as are described explicitly when using a systems dynamic approach (see Chapter 5).

6.6 L-V vs Systems Ecology

There are several assumptions made for the L-V model most, if not all, of which are not readily acceptable with a knowledge of ecology and trophic dynamics.

Most obviously, there is no linkage in terms of material transfer between predator and prey (the equations for predator and for prey use units that do not “talk” to each other at all; there is no common currency such as gC), there is no recycling of resources, and indeed no resource limitation on the prey. There is no stated maximum rate of predator growth, no assimilation efficiency, and no respiration. Why does this matter? It matters because both quality and quantity of resource critically affects ecological function, as per ecological stoichiometry (Sterner & Elser 2002; Mitra & Flynn 2006a).

In short there are key features of reality that a biologist may expect, and are fundamental drivers in ecology, which are absent from these traditional models. None of these issues has prevented the L-V model from being used countless times for applied and theoretical applications across a range of topics. It is important to appreciate that L-V was developed at a time when understanding and computational abilities were very limited; as understanding develops one may expect descriptions (conceptual and mathematical) to develop as well (see Section 6.8).

6.7 Things to Explore with L-V Models

- i) Run the L-V model using different time-step sizes using Euler or RK routines. Compare with the behaviour of the predator-prey model developed in Chapter 5 using Euler vs RK; which model is more robust and why?

- ii) Compare the behaviour of the L-V model with the predator-prey model from Chapter 5, noting that the latter contains a resource that constrains growth of the prey, while the L-V model does not.
- iii) Vary the L-V constants; what happens to the dynamics?
- iv) Should parameter “ k_3 ” be allowed to exceed, or even equal “ k_2 ”? If so, under what types of situation may that be possible?
- v) How would you measure the values of the constants in Table 6.2? Do they have any real biological meaning, or are they akin to statistical fitting parameters?
- vi) What biological factors are missing from the L-V model?
- vii) How does the L-V model structure relate to the logistic equation?

6.8 A Commentary on Empirical vs Mechanistic (Trait-Based) Models

Logistic and L-V models are “**empirical**” descriptions. That is, they may describe the dynamics of reality but they do not necessarily explain how and why it functions as it does. This is particularly obvious with Logistic and L-V constructs, where there is no resource limitation, or for L-V which lacks any explicit biologically-justified feedback interaction.

Empirical models are usually simple, if not extremely simple. That simplicity may render the equations amenable to solving through formal mathematical analysis; that is perhaps their greatest attraction. Complex models are usually only solvable numerically (i.e., using an integration routine). For example, with a complex model determining the concentration of a resource that provides a certain biological output requires the model to be run with different (or differing) resource concentrations until the required output is provided. But at least you can do it; with a Logistic Equation model there is no resource. We will return to this issue in tuning (optimisation) in Chapter 14.

In contrast to using empirical models, you could use “**mechanistic**” descriptions. These contain equations whose formulation attempts to mimic the mechanistic basis of real systems. In biological systems interactions are dominated at all stages and levels (biochemistry in a cell through to planet scale ecology) by complex series of feed-back, and also feed-forward, processes. Accordingly, it may be argued that descriptions of biological systems with an explicit inclusion of appropriate feedback processes (which are after all defining features of the functioning of all life on Earth) are required to justify a “mechanistic” tag.

The construction and deployment of mechanistic models (i.e., models containing feedback descriptions controlling simulated behaviour of biological entities) has a greatly enhanced potential to extend our understanding of the real world than can empirical models. That said, there are several important caveats that should be recognised.

Firstly, mechanistic models need not be any better at describing real events (as determined by the match of model output against real data). Mechanistic models are also inevitably significant simplifications of reality, and there is much scope for those simplifications to be flawed in concept. A little knowledge can indeed be a dangerous thing. Failings may be at the conceptual and execution level and not necessarily simply attributable to the mathematics *per se*.

It should also be noted that even the most complex of mechanistic models contain various levels of empirical descriptions. The resource limitation that we have used hitherto, based on the Monod

approach, may be argued as mechanistic in that it resembles the Michaelis-Menten enzyme kinetics which lay at the base of transporter-mediated nutrient uptake. However, this still represents a significant simplification both with respect to the potential for nutrient diffusion to be limiting uptake at the cell surface, and the regulation of nutrient transporters by (de)repression processes within the cell.

Another way of looking at what defines a mechanistic model is whether it describes or involves functional phenotypic traits. Mechanistic models may thus also be referred to as **Trait-Based Models**. Traits, as characteristics, define organisms; some of those characteristics may most likely be of no consequence in a model (such as coloration, perforations on a diatom valve, or swimming appendage shape), while others are most certainly of consequence. Obvious functional traits (functional in terms of affecting ecophysiology) include maximum growth rates, half saturation constants, allometric features (dimensions and features that can be directly related to allometry such as biomass density, motility etc.), maximum chlorophyll content, etc.

Some researchers attempt to generate overarching trait-themes to guide modelling (e.g., Andersen et al. 2016); great care must be exercised in exploiting such approaches as there are very many exceptions to the “rules”, as is usually plain from the log-log plots (e.g., of size versus maximum growth rate) presented to support the said “rules”. Great care is also required when selecting the mathematical functionality used to embed a trait into a model (e.g., Mitra & Flynn 2016; Flynn et al. 2018). The embedding of the selected mathematical function also need not be mechanistic from a biological viewpoint. Thus, an abrupt cessation of feeding could be described upon satiation of a predator, rather than employing a sigmoidal curve to gradually decrease the feeding rate as satiation is approached (as would be consistent with biological feedback mechanisms). Another example is the rate of acclimation simulated in models; a model that takes days to attain a acclimated condition when in reality it should be accomplished in hours will not describe the overall dynamics correctly (e.g., Flynn et al. 2001).

None of the above facets of real biological and ecological systems may be simulated using Logistic or L-V approaches. Other than the Logistic and Lotka-Volterra models, all other descriptions in this book can be considered as being mechanistic or trait-based to some extent or other.

6.9 Dysfunctionality and When Models Go Wrong

Ultimately, what is arguably more important than whether a model is based on this or that philosophy is whether the simulation displays **dysfunctionality**. That is, do any of the subcomponents, or combinations of them, describe events that run contrary to expectations during simulations?

For example, if you take the L-V model described above and ran it to represent a situation with no predators, then it just shows prey growth continuing for ever. In reality the prey must run out of resources. The Logistic Equation does describe density dependence in growth; but it is based solely upon an increasing mortality rate with increasing population abundance, without reference to what those factors may be (resource limitation, lack of space, infections, etc.).

It may be argued that all models are wrong but some are useful (attributed to the statistician Sir George Box; see Section 1.4). The saying is usually considered as a blanket condemnation of all models, rather than to just statistical approaches for which Box made his reputation. Here we

consider non-statistical, systems dynamics, models. While some such models are most certainly wrong, there is no reason why they should all be wrong. A model that is held to be wrong should not be used. To be wrong means it is incorrect – it is dysfunctional (see Flynn 2005a for a full discussion on this terminology). All simplifications must include omissions; the question is whether the absence of certain features causes dysfunctionality when the model is operated within a given scenario, and also whether those aspects that are included are themselves dysfunctional.

Indeed, as a model is a simplification of reality, then the first question is whether our understanding of reality is itself sufficiently complete to enable us to judge how/where to simplify and thence commence construction of a model. Very often our ability to build a model is constrained because of the unavailability of data collected using appropriate methods, and in appropriate units, as well as a lack of conceptual understanding.

6.10 Where Next

You have now built a few models; it is time to make things more complex. We have previously explored (Chapters 4 & 5) interactions between nutrient-resource limitation and predator-prey interactions and nutrient cycling. In this Chapter we considered purely empirical descriptions of density dependence. There are two obvious density dependant processes that we need to consider in connection with plankton ecology. One is the self-shading that develops within developing phytoplankton blooms (Chapter 8), and the other is what is termed intra-guild cannibalism in which, at high animal abundances, members of the same functional group turn on each other. A simple version of this, termed the closure term, is described in Chapter 11. First though, in Chapter 7, we consider dilution events.

7. Changing the Environment – using Dilutions

Terms and concepts introduced in this chapter- chemostat, turbidostat, harvesting, up-shock, down-shock, acclimation

7.1 Ecological Context – the Importance of Dilution Events

Very few real systems operate in a closed environment, akin to a culture system in a sealed flask. The most obvious feature of real environments is that they are not closed, that they have an exchange in and out of the system, transferring material with adjoining environments. Think of a lake ecosystem, for example, with inputs from rain water, from rivers and off the land, and outputs to evaporation, leakage into the sediment, and outflowing rivers.

In laboratories, experiments are most easily conducted using a flask operating essentially as a sealed, closed, system. Alternatively, experiments may be conducted in a system called a **chemostat**. A chemostat is a vessel in which the liquid volume stays constant, with the flows of material in and out occurring at the same rate. Operation of a chemostat could be likened to a pond with streams entering and leaving but with the pond remaining of constant volume.

The **inflow** brings in fresh medium containing resources (usually just nutrients, though it could contain prey); one of those resources is chosen by the experimenter to limit growth of organisms in the vessel.

The **outflow** removes medium containing residual resources (i.e., those not consumed), any materials released by the organisms and not re-assimilated, and also the organisms growing in suspension.

The proper functioning of a chemostat requires that the contents of the vessel are well mixed. Notably, organisms must not be growing adhered to the vessel wall, and they must also be growing in an asynchronous state (i.e., organisms are at all different stages of their life cycle). Assuming these conditions are met then the organisms grow within, and are washed out of, the vessel in a constant, consistent, fashion.

The dilution rate (in and out) dictates events within the chemostat. Once the system has reached an equilibrium, where everything is in steady-state (see Chapter 4), then **the dilution rate is equal to the growth rate** of the organisms. At steady-state, where dilution rate dil equals growth rate u , growth rate is limited by the residual concentration of the limiting resource. If dil is greater than the maximum possible growth rate for the organisms within the vessel then the organisms are washed out.

As we shall see, the relationship between these dilution rate and residual nutrient concentration is non-linear. Actually growth in chemostats at different values of dil provides a route to obtaining the relationship between the resource concentration (which here is the residual resource concentration in the chemostat vessel) and growth rate (because $u = dil$); after analysis of the experimental data we could obtain the values of the constants used in the Monod equation (see Chapter 4). It was by tracking microbial growth in a nutrient-limited chemostat that Monod (1949) formulated what we term the Monod equation. In traditional format this description of growth appears as:

$$\mu = \mu_{max} \cdot \frac{S}{S+k_g} \quad \text{Eq.7.1}$$

Here, S is the resource concentration, k_g is the value of S that enables $\mu = \mu_{max}/2$; k_g is thus the half saturation constant. Note that S is the residual concentration in the chemostat; it is not the concentration of the nutrient in the inflow medium. The equation (Eq.7.1) is in essence exactly the same as the Michaelis-Menten equation for enzyme activity we saw in Chapter 4 (Eq.4.2).

As a linear equation for use in model code, Eq.7.1 may appear like this:

$$u = u_{max} * S / (S + k_g) \quad \text{Eq.7.2}$$

For a chemostat, we set different values of μ (via the dilution rate, dil) and obtain the value of S . By using an iterative curve fitter, or one of the classic linear transforms of the Michaelis-Menten equation (such as the Hanes-Woolf plot, of S against S/μ), we can obtain values for μ_{max} and k_g .

There are other types of culture 'stat; most importantly for plankton work there is the **turbidostat** which operates to maintain a set desired concentration of organisms. Here the pumps for inflow and outflow are controlled by the optical density (colour) of the suspension, switching on when organism abundance (and hence optical density) attains a set required value. In contrast, within a chemostat the pump operates all the time; in consequence there is a distinct risk at values of dil approaching the maximum growth rate that the organisms will be washed out because even well mixed suspensions of asynchronous organisms sometimes exhibit a hiccup in their growth dynamics such that $\mu < dil$. Such a washout event should not occur in a turbidostat as the pumps will turn off if the optical density goes low.

As mentioned above, in nature, water bodies are also subjected to inflow and outflows. This is obvious in a lake, pond or reservoir (see Chapter 10 for a model). Dilution rates may be high in such systems; at the extreme the system is more like a river, with a very high dilution rate (which is the primary reason why plankton do not grow in most rivers – their growth rate cannot match the dilution rate).

Dilutions can also be considered to occur in the oceans, where there is an exchange across the mixed layer that brings in nutrient rich water from the depths and removes surface water containing organisms and residual nutrients and chemicals released by the biota. These dilution rates across the mixed layer are typically slow (ca. $< 0.05 \text{ d}^{-1}$; see Chapter 12), much slower than usually operated within a chemostat. In a chemostat, typically dil is some significant fraction of the maximum growth rate, at around ca. $0.2 - 0.5 \text{ d}^{-1}$ for phytoplankton cultures.

In food web microcosms running in chemostats, it may be tempting to assign some additional meaning to dilutions (such as losses due to predation) in addition to that resembling mixing events. However, it should be noted that dilution of a whole population (simultaneous and equal removal rates of all food web components and nutrients) is not representative of what are usually selective feeding events exhibited by grazers such as higher trophic organisms in a real ecosystem.

In this chapter we will explore the consequences of dilution approaches on the dynamics of modelled systems. There are often occasions in laboratory studies, and also in commercial growth of phytoplankton, where a large fraction of a culture (e.g., 95%) may be removed during harvesting, and the volume replaced with fresh medium. Such an event greatly disturbs the steady-state dynamics, creating an **up-shock** to the system. An up-shock is an event that relieves stresses or limitations to the organism, while a **down-shock** occurs on exhaustion of resources.

These up- and down- shocks are associated with biochemical events termed **acclimations**, during which organisms realign their physiology to best exploit or survive the new conditions. (Note that many researchers incorrectly term such acclimations as “adaptations”; the former occurs within generations while the latter is intergenerational and involves evolutionary processes.)

7.2 Simulating the Chemostat

We start here by using as a base the simple phytoplankton model we developed in Chapter 4. To this model we need to add inflows and outflows, which will operate with a given dilution rate set by *dil*.

First, an explanation of units. The model we built previously (Chapter 4) was a N-biomass-specific description. Concentrations of both the resource (ammonium, *Am*) and the organism (phytoplankton, *Phy*) carried units of $\mu\text{gN L}^{-1}$. The units of dilution, *dil*, are $\text{L L}^{-1} \text{d}^{-1}$; for every L of volume, a certain volume is added and removed per day; note that the dilution process is continuous in a chemostat, in the same way that growth in continuous light will be a continuous process for the phytoplankton. What we are concerned with, however, is not just the flow of growth medium as much as with what is in the medium.

For *Am*, there is a flow in and out; for *Phy* there is just a flow out. That is to say, the ammonium concentration in the chemostat reflects both addition of ammonium and its washout, and also the removal of ammonium through uptake into the phytoplankton biomass. The phytoplankton biomass increases in consequence of using ammonium, and decreases with dilution as some proportion of the biomass is washed out. Let us now consider these in detail.

Inflow

The inflow of medium brings in ammonium. This comes in at a stated concentration as set by that in the growth medium pumped in from an external reservoir. So we need in addition to *dil*, the concentration of ammonium in that external reservoir; let us define this by the constant, *ext_Am*. This has the same units as *Am*, as $\mu\text{gN L}^{-1}$. The rate of inflow of fresh resource (*in_Am*; $\mu\text{gN L}^{-1} \text{d}^{-1}$) is thus given as:

$$in_Am = ext_Am * dil \quad \text{Eq.7.3}$$

Outflows

The medium that is pumped out carries with it a fraction of the residual ammonium, plus the same fraction of the biomass (noting that the liquid volume in the vessel remains the same). The fraction is, of course, set by *dil*.

For ammonium we have:

$$out_Am = Am * dil \quad \text{Eq.7.4}$$

For phytoplankton biomass we also have a removal by dilution:

$$out_Phy = Phy * dil \quad \text{Eq.7.5}$$

We could combine the flows for *Am* to describe the net inflow of ammonium (*netin_Am*), thus:

$$netin_Am = dil*(ext_Am - Am) \tag{Eq.7.6}$$

The value of *netin_Am* (as $\mu\text{gN L}^{-1} \text{d}^{-1}$) should be the same as *out_Phy* at steady state, as the missing ammonium-N is within the phytoplankton biomass.

7.3 The Model

The modified model appears as in Fig. 7.1, with equations in Table 7.1

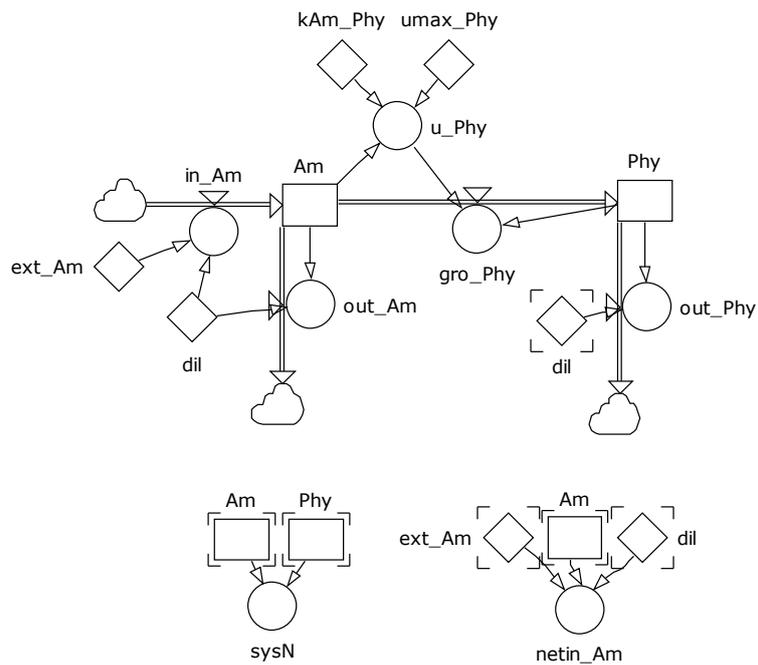


Fig. 7.1 Chemostat model for N-limited growth of phytoplankton.

| Parameter | Type | Value | Unit | Description |
|-----------------|------|---|-------------------------------------|--|
| <i>Am</i> | SV | 99 + <i>in_Am</i> - <i>out_Am</i> - <i>gro_Phy</i> | µgN L ⁻¹ | Ammonium-N |
| <i>Phy</i> | SV | 1 + <i>gro_Phy</i> - <i>out_Phy</i> | µgN L ⁻¹ | Phytoplankton biomass-N |
| <i>dil</i> | Con | 0.2 | L L ⁻¹ d ⁻¹ | Dilution rate |
| <i>ext_Am</i> | Con | 100 | µgN L ⁻¹ | Concentration of <i>Am</i> in external reservoir |
| <i>kAm_Phy</i> | Con | 14 | µgN L ⁻¹ | Half saturation constant for <i>u_Phy</i> |
| <i>umax_Phy</i> | Con | 0.693 | gN gN ⁻¹ d ⁻¹ | Phytoplankton maximum N-specific growth rate |
| <i>in_Am</i> | Aux | <i>ext_Am</i> * <i>dil</i> | µgN L ⁻¹ d ⁻¹ | Inflow of <i>ext_Am</i> from reservoir |
| <i>u_Phy</i> | Aux | $\frac{umax_Phy * Am}{Am + kAm_Phy}$ | gN gN ⁻¹ d ⁻¹ | Phytoplankton N-specific growth rate |
| <i>gro_Phy</i> | Aux | <i>u_Phy</i> * <i>Phy</i> | µgN L ⁻¹ d ⁻¹ | Phytoplankton population growth rate |
| <i>netin_Am</i> | Aux | <i>dil</i> *(<i>ext_Am</i> - <i>Am</i>) | µgN L ⁻¹ d ⁻¹ | Net input of <i>Am</i> |
| <i>out_Am</i> | Aux | <i>Am</i> * <i>dil</i> | µgN L ⁻¹ d ⁻¹ | Outflow of <i>Am</i> from culture vessel |
| <i>out_Phy</i> | Aux | <i>Phy</i> * <i>dil</i> | µgN L ⁻¹ d ⁻¹ | Outflow of <i>Phy</i> from culture vessel |
| <i>sysN</i> | Aux | <i>Am</i> + <i>Phy</i> | µgN L ⁻¹ | System N-balance |

Table 7.1 Equation set modified from Table 4.1, with addition of chemostat dilution. The value for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

The initial values of *Am* and *Phy* should ideally be set to sum to the value of *ext_Am*. If this is not done then the value of *sysN* will take some time (depending on the dilution rate and the disparity) to converge to match the value of *ext_Am*.

If possible, configure your software to enable the values of *dil* and *ext_Am* to be altered during a run. This may require the software to pause every so many time steps and await a response from you. This will enable you to undertake an *in silico* experiment similar to an empirical study of the effects of altering the chemostat operational parameters on the biomass yield and production rates.

The code for such a control could read something like this –

$$\text{PAUSEIF}(\text{FRAC}(\text{TIME}/\text{Pause_time})=0) \quad \text{Eq.7.6}$$

Here the period between pausing is set by *Pause_time* (e.g., 10 days). The run is paused when the value of simulation time (*TIME*) divided by *Pause_time* is a whole number, with no fraction (i.e., *FRAC* = 0).

Examples of model output are given in Figs. 7.2 – 7.4.

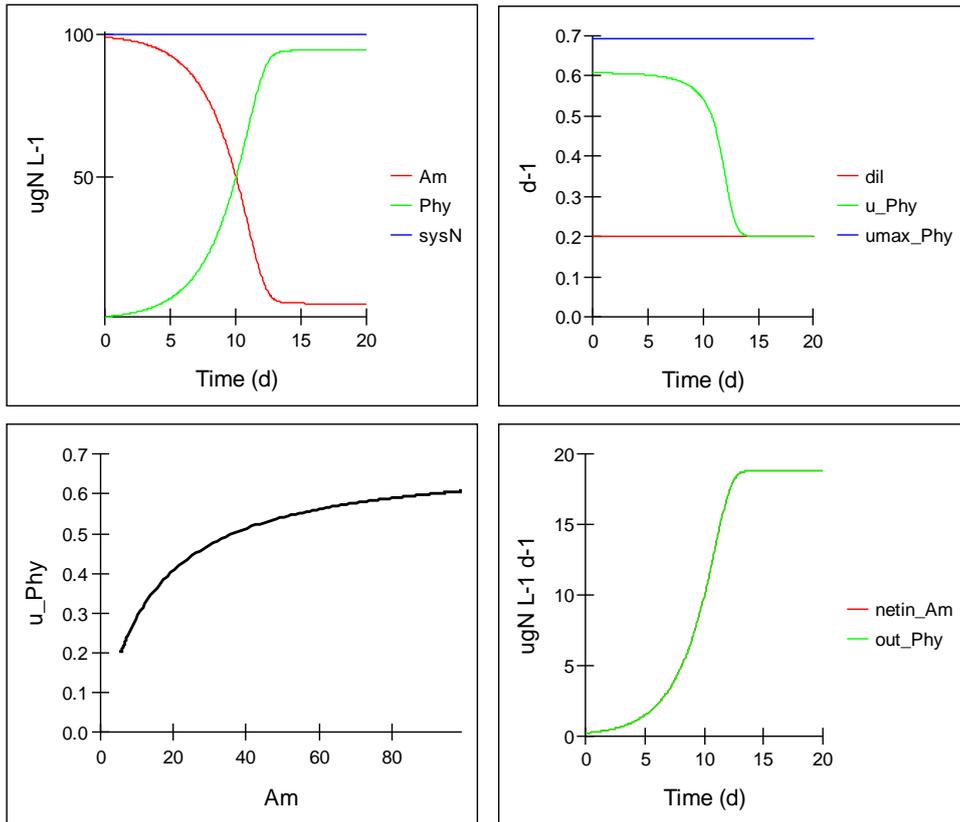


Fig. 7.2 Simple model operation with $dil = 0.2 \text{ d}^{-1}$ showing initial batch-culture like dynamics. Note that as long as sufficient resource (Am) is available then u_Phy exceeds dil ; by time 12, the value of Am has been consumed down to a critical value at which u_Phy matches dil . Over this time the relationship between Am and u_Phy describes a rectangular hyperbola which here, with $dil=0.2$, matches $u_Phy = 0.2$.

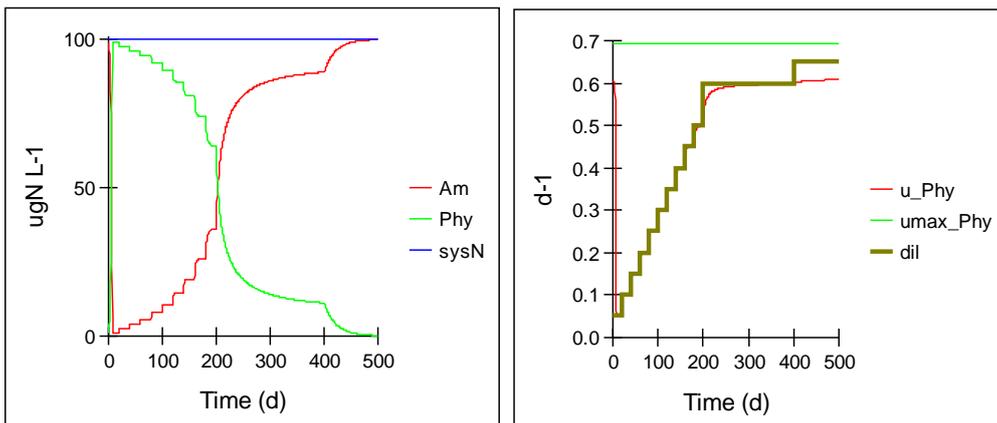


Fig. 7.3 Model operation with dil altered sequentially from 0.05 to 0.65 d^{-1} . As dil is increased so u_Phy increases to match; however, this can only occur at increasingly high external residual concentrations (Am). Note that u_Phy cannot closely approach $umax_Phy$ because the concentration of ext_Am in this particular system is ultimately limiting the growth rate significantly, and so when $dil > 0.6 \text{ d}^{-1}$ the organism is washed out.

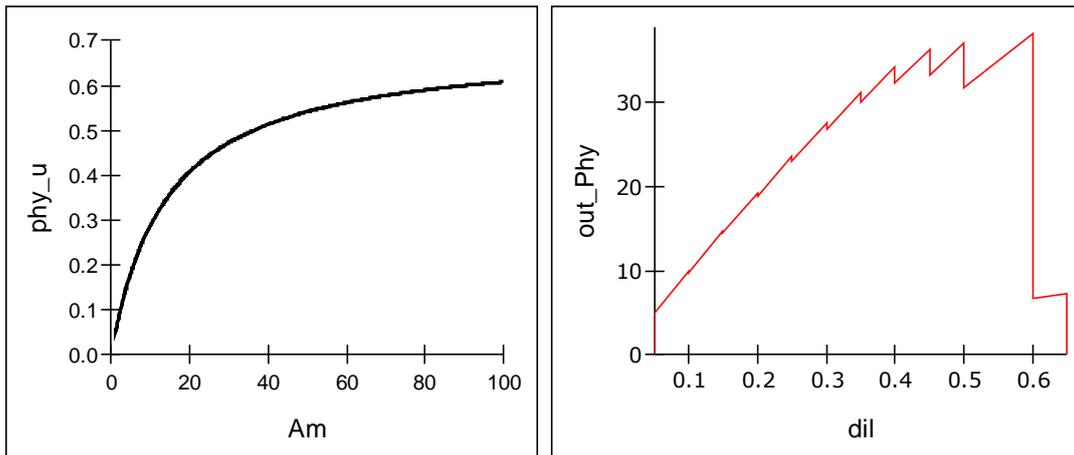


Fig. 7.4 Plots of the relationship between resource (Am) and growth rate (u_{Phy}), and between dilution rate (dil) and harvestable rate (out_{Phy}) from the simulations shown in Fig. 7.3.

7.4 Simulating Culture Harvesting

Often a batch culture, or indeed a continuous culture system such as a turbidostat or chemostat, will be subjected to a significant harvest in which a large proportion of the culture volume will be removed over a short period of time.

It should be noted that under standard operations there is a steady but typically low volume of culture pumped from a continuous culture system that is likely insufficient to work with (for biochemical analysis, for example). During a harvest, a larger proportion of the culture will be removed, and the volume replaced with fresh medium. This suddenly provides a significant increase in residual nutrient concentration, and the organism growth rate will increase before slowing back down to match the dilution rate. The organisms would be subjected to up-shock, and then down-shock. For the purpose at hand, let us consider that the harvest event is instantaneous, or that it occurs within a single integration time-step period (which for most of these models will equate to a few 10s of minutes, which actually is indeed not dissimilar to the time taken to harvest a real culture system of a few 10s of litres).

To handle this simulation, firstly there is the issue of the trigger for the event, secondly there is the issue of the dilution rate itself.

The trigger can, as in reality, be set by various routes. The most obvious alternatives are:

- Every so-many days, a set % of the system is harvested.
- Harvesting of a certain % occurs once the residual nutrient load falls below a stated threshold or that the biomass concentration exceeds a certain threshold. (In reality nutrients could be measured continuously using a suitable ion-specific electrode, or biomass could be monitored as for a turbidostat.)
- On demand.

One could imagine for a commercial operation the trigger and the % harvested could be optimised to secure the highest biomass yield, or perhaps the largest nutrient recovery.

The trigger needs to be installed using some form of switch, using an IF-THEN-ELSE construct.

The following (Fig. 7.5, Table 7.2) installs a switch to harvest a set % of the culture at a set frequency.

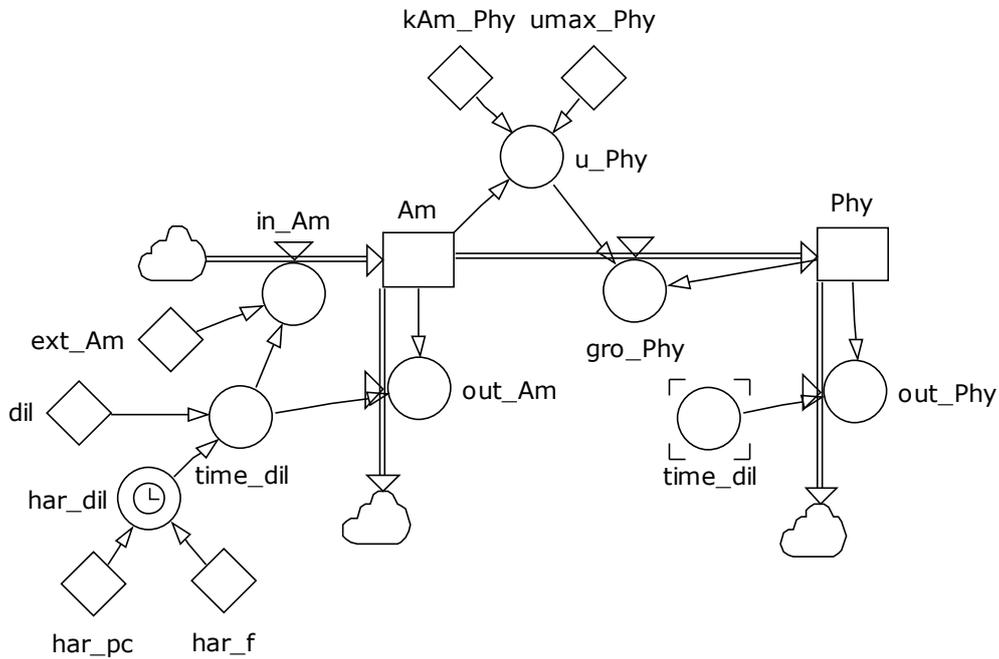


Fig. 7.5 Modified model with harvesting function. See Table 7.2.

| Parameter | Type | Value | Unit | Description |
|-----------------|------|---|-----------------|---|
| <i>dil</i> | Con | 0.2 | d ⁻¹ | Background dilution rate |
| <i>har_f</i> | Con | 20 | d | Frequency of harvesting |
| <i>har_pc</i> | Con | 0.95 | dl | Proportion harvested at frequency of <i>har_f</i> |
| <i>har_dil</i> | Aux | IF((TIME>0), 1, 0)*IF((FRAC(TIME/har_f)=0), 1, 0)*har_pc/TIMESTEP | d ⁻¹ | Harvesting dilution rate |
| <i>time_dil</i> | Aux | <i>dill</i> + <i>har_dil</i> | d ⁻¹ | Total dilution rate |

Table 7.2 Harvesting function equations. See also Figs. 7.1 and 7.5. dl – dimensionless.

The explanation of the equation for *har_dil* in Table 7.2 is as follows: Assuming that simulation time is greater than 0 (i.e., not at the start) then harvesting occurs when the time is a simple multiple of *har_f*; that condition occurs when the simulation time is an exact multiple of *har_f*, and hence when the fraction of TIME/*har_f* is zero. When these conditions are met then harvesting occurs. At that precise time, a proportion of the system, set by *har_pc*, is removed. Because the event occurs over a single time-step the effective dilution rate is set by *har_pc*/TIMESTEP.

NOTE: this will only work using the Euler integration routine; it will not work correctly using R-K routines (see Chapter 2, Section 2.6).

Example outputs are shown in Fig. 7.6.

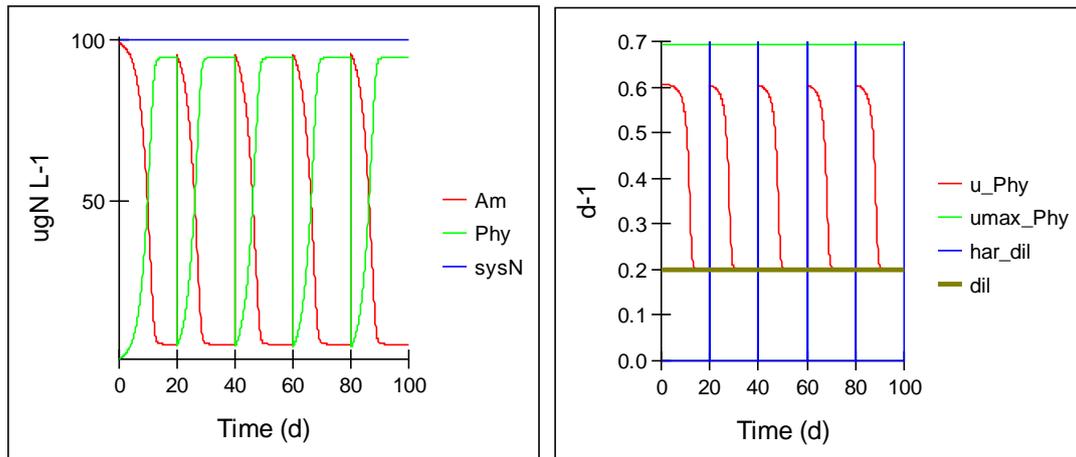


Fig. 7.6 Output using the harvesting component. Here, every 20 days 95% of the system is diluted out at a harvest event ($har_pc = 0.95$). The phytoplankton growth rate (u_Phy) changes over that time, increasing sharply with the up-shock event. u_Phy has a minimum value set by dil ; although the residual nutrient concentration (Am) is low, the supply rate prevents extreme nutrient starvation from developing.

7.5 Parameterising the Models

Parameterisation of the models is the same as for the base model described in Chapter 4. However, now the systems are being run into steady-state (down-shock), during steady-state, or being perturbed from steady-state (up-shock).

It can take many generations (weeks) for a real population to attain true steady-state. Once in steady-state sampling can be taken at any periodicity and the physiological status of the organisms should (by definition) be the same. Most obviously, growth rate will equal dilution rate. However, when parameterising changes in behaviour during times other than steady-state (during up-shock or down-shock), samples need to be taken very frequently; running your model before conducting the experiment (which is rather like operating a dynamic hypothesis test-bed) can guide you in selecting time points of likely interest for sampling your experimental system.

Be aware that while in theory a chemostat provides an endless supply of biological material in an identical physiological state, in practice there are two important logistical hurdles:

1. A large volume of reservoir medium is required for operating even a small chemostat system; if you wish to explore that with your model you need to construct a parallel description of the culture volume, and account for the volumetric flows in and out of the chemostat itself.
2. While there is indeed a ready availability of culture material, the actual amount of material is very small (as a function of the dilution rate and the volume of the chemostat). If you need a respectable volume of culture then most likely the volume will be disturbed significantly (as in the harvesting simulation shown above; Fig. 7.6), and the system will take some time to return to true steady-state.

You can explore these challenges by using the harvest model – see how much you can remove in one time interval and what the implications are for system dynamics.

7.6 Things to Explore

- i) Configure the predator-prey model from Chapter 5 for a chemostat operation. To do that, you need to identify the components in the chemostat model that describe the dilution process, and build them into the predator-prey model. Note that you need a dilution out of the zooplankton state variable, analogous to that from the phytoplankton state variable. Set the zooplankton biomass to 0, and observe what happens to the growth rate, phytoplankton biomass and residual nutrient loading at different dilution rates – it should be the same as you see using the model shown in Fig. 7.1 for a given set of input constants.
- ii) From (i) now introduce the zooplankton (i.e., set the initial zooplankton, Z , at some value), and repeat. Note that the zooplankton and phytoplankton are both subjected to losses incurred through dilution. *De facto*, because of the inflow of fresh nutrient, there is an event akin to a simultaneous regeneration of N from these dilution-inspired biomass losses. Explore how changes in growth rates and feeding parameters affect the success of the phytoplankton vs the zooplankton.
- iii) The model in (ii) is a “green” culture system; you could build a two-phase culture system, in which a chemostat for the phytoplankton is coupled to another for the zooplankton. You thus have two dilution rates to adjust.
- iv) Explore the implications of different harvesting rates on the steady-state dynamics.
- v) Rebuild the models to act as a turbidostat, in which the rate of dilution is adjusted to maintain a set biomass in the culture vessel. The easiest way to do this is to make the value of dil a function of the value of biomass concentration and a reference (target) concentration. This can be configured as a simple on-off switch referenced to Phy attaining a critical value, setting $dil = 0$, or $dil = umax$.

7.7 Caveats

- Caveats apply to the component models of the organisms simulated to be growing within the chemostat just as they do for batch culture systems (see Chapters 4 and 5).
- Note that a turbidostat can be used to generate a culture in a non-limited nutrient status, while a chemostat requires that a nutrient is limiting. You may think that you could thus grow a pea-soup culture at high rate in a turbidostat, but there is another important “nutrient” that will become limiting, and that is light. This causes self-shading of the phytoplankton. As we shall see in Chapter 8, this has a major impact on the dynamics of growth. This is further affected by the degree of photoacclimation and the interaction with nutrient status which collectively affect the amount of photopigment in the cells and thence how “green” is the culture. This can be an important factor in the commercial growth of microalgae (Kenny & Flynn 2015, 2016).

7.8 Where Next

In this consideration of chemostat operation, no regard is given to the self-shading that develops within a dense phytoplankton (microalgal) culture. And that shading will be removed if a predator grows in the system as well. This can give a complex, series of interactions. The topic of self-shading and the impact on photosynthesis is explored further in Chapter 8.

8. Density Dependence – Light Limitation and Self-Shading

Terms and concepts introduced in this chapter- self-shading, photoacclimation, PE curve, depth-integrated photosynthesis

8.1 Ecological Context

In previous models we have described the control of phytoplankton growth through single nutrient limitation. In reality, most often light at least co-limits phototrophic growth. Sometimes that is due to too much light, which then causes photodamage and/or photoinhibition, and perhaps even kills cells. Typically though, the limitation is due to a lack of light. Furthermore, there is a positive feedback interaction involved with low-light limitation because through the process of photoacclimation (commonly, though incorrectly, referred to as “shade-adaptation”, for example in reference to house plants) the individual organism becomes more heavily pigmented.

In crude terms each photoautotrophic organism becomes greener as it acclimates to capture the decreasing number of photons available, and so the ratio of chlorophyll to biomass, which we may describe as Chl:C, increases towards a maximum. The consequence of each member of the phytoplankton population becoming more densely pigmented, plus the increase in the population size, rapidly leads to a decrease in the amount of energy being available to the individual, and hence to a decrease in specific growth rate.

The process of light limitation of growth can be seen to have several facets. The surface irradiance may itself, even for cells at the water surface, be too low to permit high rates of photosynthesis. And of course light varies over the course of the day, with cloud cover and with the day-night cycle. Then, as the population grows, the light available to the individual declines as the sum total of pigment increases. And then we add in the aforementioned photoacclimation, where the ratio of chlorophyll pigment to biomass changes.

Here, although we shall consider the simplest scenario in which we ignore photoacclimation (assuming a set fixed Chl:C), we will explore how nutrient loading, mixing depth of the environment and irradiance all interact to affect the emergent growth rates of the individual and of the population.

8.2 The Basics of Photosynthesis

Photosynthesis is a complex process, but at its simplest the relationship between light and photosynthesis may be described by a photosynthesis-irradiance (**PE**) **curve**. Some older texts term this a “*PI curve*”, but “*I*” has been claimed by physicists for amps, and *E* is used for irradiance.

The process of photosynthesis, and hence the *PE* curve, exhibits two main features.

1. At low light there is an essentially linear section with gradient α (*alpha*); this donates the efficiency with which energy as photons is used to generate photo-reductant, which enables CO₂-fixation, and thence eventually supports biomass-growth.
2. Then there is a plateau which reflects the maximum scope for photosynthesis (*PSmax*).

The organisms that undertake this process are themselves (as plankton) living within a body of water, exposed to different levels of irradiance depending on their depth. The water itself, plus the suspended organisms, collectively attenuates the amount of light received, averaged over time, and thence affect what is termed the *time and depth integrated* level of photosynthesis.

To describe all this in full detail would be most comprehensively achieved using a model that described for individual cells (or clusters thereof – see Section 2.9) their exposure to light as they move through the water column, and the total of those exposures and subsequent activities would describe the population process. This is complex both from a modelling standpoint, and also computationally. Fortunately, there is a simplified approach that is quite adequate for most applications (e.g., Kenny & Flynn 2015, 2016). The caveat is that we must assume that cells are indeed moving around throughout the mixed depth in a random and homogeneous fashion.

There are various empirical descriptions of the *PE* curve, but the only one that can be integrated analytically is the equation of Smith (1936). The Smith equation itself (as configured for our purpose) describes the rate of photosynthesis (*PS*) as:

$$PS = PS_{max} * (1 - \text{EXP}(-\alpha * ChlC * E / PS_{max})) \quad \text{Eq.8.1}$$

The value of *alpha* here has units of (m² g⁻¹ Chl)*(gC μmol⁻¹ photon), *ChlC* is the mass ratio of cellular chlorophyll to cell-C, and irradiance *E* is the daily light dose. *PS_{max}* is the maximum rate of gross photosynthesis, that is to say, ignoring the respiration which generates CO₂ rather than fixing it. *PS* minus respiration describes net photosynthesis; assuming no leakage of photosynthate (as sugars, for example), the net photosynthetic rate equates to the growth rate. Gross photosynthesis is zero when PFD=0; net photosynthesis is negative when PFD=0 and does not become zero until some critical amount of light is made available (the “compensation point”, where *PS* = respiration).

As we shall describe shortly in more detail (in Section 8.3), light can be described in various units but, to be consistent with the units of *alpha* that we have just declared, we describe light as photon flux density (*PFD*) with units of μmol photon m⁻² s⁻¹. This means that so-many micromoles of photons hit an area of 1 m² per second. However, here we need the dose in time units of day, so *E* is given as *PFD* × 60 × 60 × 24, thus giving units of μmol photon m⁻² d⁻¹.

In total then, the units of *alpha***ChlC***E* thus collapse to d⁻¹. The units for *PS_{max}* are also d⁻¹, so the units of the exponential (EXP) part of Eq.8.1 is dimensionless, so the unit for *PS* given by Eq.8.1 is the same as *PS_{max}* (which is as it should be!).

If we set the following values then the *PE* curve appears as in Fig. 8.1; *alpha* = 3E-6, *ChlC* = 0.03, *PS_{max}* = 1, *PFD* as μmol photon m⁻² s⁻¹. It is instructive to explore what happens when you alter the values of *alpha* (try 1E-6 to 10E-6), *ChlC* (try 0.005 to 0.08), and *P_{max}* (try 0.25 to 3). Note this is gross photosynthesis, with no account taken of any concurrent respiration that would make the (net) value of *PS* negative in darkness. It should also be noted that this is an instantaneous relationship, akin to that a physiologist might measure in very short-duration ¹⁴CO₂-fixation or O₂ evolution experiments (correcting for respiration, of course). A relationship between irradiance dose and daily growth will thus look different.

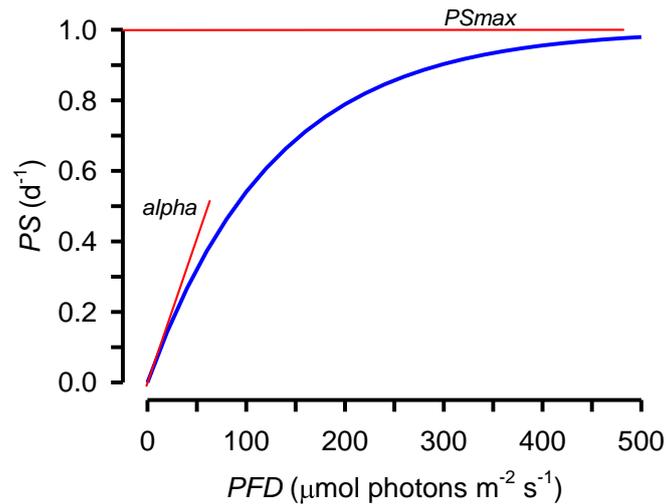


Fig. 8.1 PE curve for gross photosynthesis, showing the role of *alpha* and *PSmax* as values delimiting the shape.

8.3 Depth Integrated Photosynthesis

Parts of what follows may appear overly complex; you do not need to work your way through this section unless you are comfortable doing so. Ultimately, you only need the equations as presented in Table 8.1.

The basis of the derivation of the depth integrated form, and the description of the calculus, can be found described in Smith (1936) and also explained in Kenny & Flynn (2016); here we will just develop the application.

We start by identifying the key parameters.

First, of course, there is light. Light can be described using various units some of which are now rarely used. For plankton, light is best described in terms of power (W m^{-2}) or as photo flux density (*PFD*; $\mu\text{mol photons m}^{-2} \text{s}^{-1}$). Whatever unit you use for light you must use the reciprocal for *alpha* else the units will not cancel out. In descriptions of phototroph physiology *PFD* is the unit typically used, and this considers light over the photosynthetically active radiation (PAR) wavelength band, which is 400-700nm. This PAR, coincidentally, aligns with the visible spectrum of light for humans. A value of PAR *PFD* of ca. 2000 $\mu\text{mol photons m}^{-2} \text{s}^{-1}$ broadly equates to full midday sun; near the equator, peak values approach 3000.

Then there is the depth of the water body in which the organisms are held (*z*), or the optical depth of a flask (given that light will come from several directions simultaneously, the effective depth may be approximated as the radius of the flask). The depth is in units of m.

The water itself, devoid of organisms, has its own attenuation coefficient (*attco_W*), which carries with it the unit m^{-1} . For pure water the value will be close to 0, but natural waters invariably contain coloured material, and some waters loaded with tannins or chemicals from anaerobic digestates or decomposing leaves can be highly coloured. Let us assume typical clean culture media, with an attenuation of 0.05 m^{-1} ; a similar value can be assumed for ocean water.

To the absorbance due to the water alone, we now need to add the attenuation due to the presence of the photosynthetic organisms ($attco_Phy$; m^{-1}). Taking the main pigment as chlorophyll_a, this has an absorbance coefficient ($abco_Chl$) of $0.02\ m^2\ (mg\ Chl)^{-1}$. Here we are using a model based upon N-biomass (as developed in Chapter 4), so we need to convert this Chl-specific absorbance value to a N-specific value. To do that we need to make a few assumptions, none of which are particularly robust, but they will suffice here.

So, let us for example assume a phytoplankton N:C mass ratio of ($NC_Phy =$) 0.15, and a Chl:C mass ratio of ($ChlC_Phy =$) 0.02. We thus obtain an absorbance coefficient for phytoplankton biomass ($abco_PhyN$) according to:

$$abco_PhyN = abco_Chl * ChlC_Phy / NC_Phy \quad \text{Eq.8.2}$$

The phytoplankton biomass attenuation coefficient ($attco_Phy$) is then given by reference to the biomass of the phytoplankton population (Phy):

$$attco_Phy = abco_PhyN * Phy \quad \text{Eq.8.3}$$

To clarify the units here; $abco_Chl$ has units of $m^2\ (mg\ Chl)^{-1}$, which means that $abco_PhyN$ from Eq.8.2 has units of $m^2\ (mg\ N\text{-biomass})^{-1}$. Phy has units of $\mu g\ N\ L^{-1}$, which is the same as $mg\ N\ m^{-3}$ (there being 1000L per m^3).

So the units of $attco_Phy$ from Eq.8.3 lose reference to mgN, while $m^2 * m^{-3}$ leaves us with a final unit of m^{-1} , which is indeed the expected unit for $attco_Phy$ (it is the same unit for $attco_W$).

The total attenuation (att_tot ; dimensionless) is a function of both the water and phytoplankton attenuations considered over the mixed layer depth (z ; m), and is thus given by:

$$att_tot = z * (attco_W + attco_Phy) \quad \text{Eq.8.4}$$

We will also need the negative exponent of att_tot ($exatt$):

$$exatt = EXP(-att_tot) \quad \text{Eq.8.5}$$

Returning to the biology, now ...

The chlorophyll-specific value of $alpha$ is often labelled in the literature as α^{chl} , so let us code that as $alpha_Chl$. The variable $alpha_Chl$ has units of gC fixed per gChl per μmol photon per m^2 : this is better written as $(m^2\ g^{-1}\ Chl) * (gC\ \mu mol^{-1}\ photon)$.

The numeric value for $alpha_Chl$ that we will use is $7e-6$, which is a very small number, but then the photon count over a day is massive. PFD has units of time as seconds, and there are 86400 seconds per day (not that the complete day need be of light, but here let us assume continuous illumination, with no darkness at night).

We now need to convert this value of $alpha_Chl$ into a N-specific value for application to our simple N-based phytoplankton model.

Using the mass transforms suggested above (i.e., N:C = 0.15 and Chl:C = 0.02) we obtain in Eq.8.6 a value for $alpha_PhyN$ of $1.4e-7$ gN assimilated per g phytoplankton N-biomass per μmol photon per m^2 .

$$\alpha_{PhyN} = \alpha_{Chl} * NC * ChIC / NC \quad \text{Eq.8.6}$$

which of course simplifies to $\alpha_{Chl} * ChIC$. This can be seen to also be the C-specific value of α (which we could label α_C to differentiate it from α_N).

In other words, and as we have considered earlier (Section 4.5), C-specific and N-specific rates are the same assuming that N and C are being assimilated in synchrony, as must be so here as we are assuming a fixed cellular N:C. (In passing we note that this assumption would not be so if a proportion of the fixed C was lost as dissolved organic carbon, such as sugars, or mucus.)

Having established that it does not matter here whether we use C-specific or N-specific terms, let us use the term α_u to indicate in generic terms the specific slope for the PE curve, so that:

$$\alpha_u = \alpha_{Chl} * ChIC \quad \text{Eq.8.7}$$

Now we proceed to compute the depth-integrated photosynthetic rate (PSz ; d^{-1}). This is the average rate of photosynthesis performed by organisms being moved throughout the mixed layer.

As an intermediary calculation we need to combine the maximum rate of photosynthesis ($PSmax$), the total photon dose over the day (noting PFD has units of s^{-1} , and there are $24*60*60$ seconds in a day), and α_u . Thus:

$$pyt = (\alpha_u * PFD * 24 * 60 * 60) / PSmax \quad \text{Eq.8.8}$$

And then to calculate the depth integrated photosynthesis rate (PS ; here as $gN gN^{-1} d^{-1}$), using the intermediary auxiliaries pyt (Eq.8.8), att_{tot} (Eq.8.4) and $exatt$ (Eq.8.5), and $PSmax$, we use the following:

$$PSz = PSmax * (\ln(pyt + \sqrt{1 + pyt^2}) - \ln(pyt * exatt + \sqrt{1 + (pyt * exatt)^2})) / att_{tot} \quad \text{Eq.8.9}$$

This, however, gives us a light limited rate of photosynthesis, and we need to consider the potential for coupled light-nutrient limited growth. So next we need to merge this in with the N-limited description developed in Chapter 4.

8.4 Nutrient and Light Co-Limitation

It is most convenient to involve a quotient (i.e., a number between 0 and 1) to describe the potential for growth limitation by nutrient availability. Here, following from Chapter 4, we use $Am / (Am + kAm_{Phy})$ as the relationship between nutrient concentration (Am) and a half saturation constant (kAm_{Phy}).

So, firstly, let us define the nutrient status as:

$$Nu = Am / (Am + kAm_{Phy}) \quad \text{Eq.8.10}$$

On the face of it we now have 2 options, but one is incorrect. The incorrect route would be to take the value of PSz (Eq.8.9), here representing the non-nutrient-limited rate of photosynthesis, and

multiply it by the quotient that comes from the rectangular hyperbola for resource availability, thus:

$$PSqz = PSz * Nu \quad \text{Eq.8.11}$$

The (more) correct way is to modify the value of $PSmax$ by this quotient, and then compute the photosynthetic rate using a new parameter, $PSqmax$, which takes account of the nutrient-limitation. Thus:

$$PSqmax = PSmax * Nu \quad \text{Eq.8.12}$$

Now we have to rewrite (and rename) the definitions of pyt and PSz to take account of $PSqmax$, thus:

$$pytq = (\alpha_u * PFD * 24 * 60 * 60) / PSqmax \quad \text{Eq.8.13}$$

$$PSqz = PSqmax * (\ln(pytq + \sqrt{1 + pytq^2}) - \ln(pytq * exatt + \sqrt{1 + (pytq * exatt)^2})) / att_{tot}$$

$$\text{Eq.8.14}$$

So, why is the second route preferable? When phytoplankton are starved of N, they degrade proteinaceous components, and that includes RuBisCO, the enzyme for C-fixation. RuBisCO, the most important single enzyme in the cell (and indeed on Earth), is not present in such high amounts in a cell that lacks incoming N with which to assimilate the newly fixed C into amino and nucleic acids. The net consequence is that the plateau value of the PE curve (which is set by the enzymes controlling C-fixation, and thus primarily by RuBisCO) declines on N-starvation. The new value, *de facto* the operational maximum value of RuBisCO activity, is defined by $PSqmax$.

Note, however, that the slope of the PE curve (set by α) is unaffected, or certainly less affected by N-limitation. In the first (incorrect) route, the whole shape of the PE curve is affected by N-limitation, the slope and the plateau, in a coordinated fashion. This does not accord with expectations. There may be reasons for why the slope of the PE curve may decline, but it is most obviously linked to a decline in Chl:C (i.e., N-starved cells become paler, with less chlorophyll); here we cheated by fixing Chl:N, assuming a fixed Chl:C (it actually varies with PFD and N-status) and also a fixed C:N (which actually increases with N-starvation).

The above describes the calculation of gross photosynthesis, ignoring respiration. We need to include a level of background activity associated with basal respiration so that net growth is negative in darkness. Setting that basal respiration scaled to the maximum growth rate via BR_{Phy} , and the target maximum phytoplankton growth rate as $umax_{Phy}$, then to be able to attain $umax_{Phy}$, the value of $PSmax$ is given as:

$$PSmax = umax_{Phy} * (1 + BR_{Phy}) \quad \text{Eq.8.15}$$

And the growth rate, which is net photosynthesis, is then:

$$u_{Phy} = PSqz - umax_{Phy} * BR_{Phy} \quad \text{Eq.8.16}$$

Finally, the growth of the phytoplankton population (i.e., increase in Phy) requires a different definition to that we used in Chapter 4, such that:

$$gro_Phy = PSqz * Phy$$

Eq.8.17

8.5 The Model

The full model is given in Fig. 8.2, and the equations in Table 8.1.

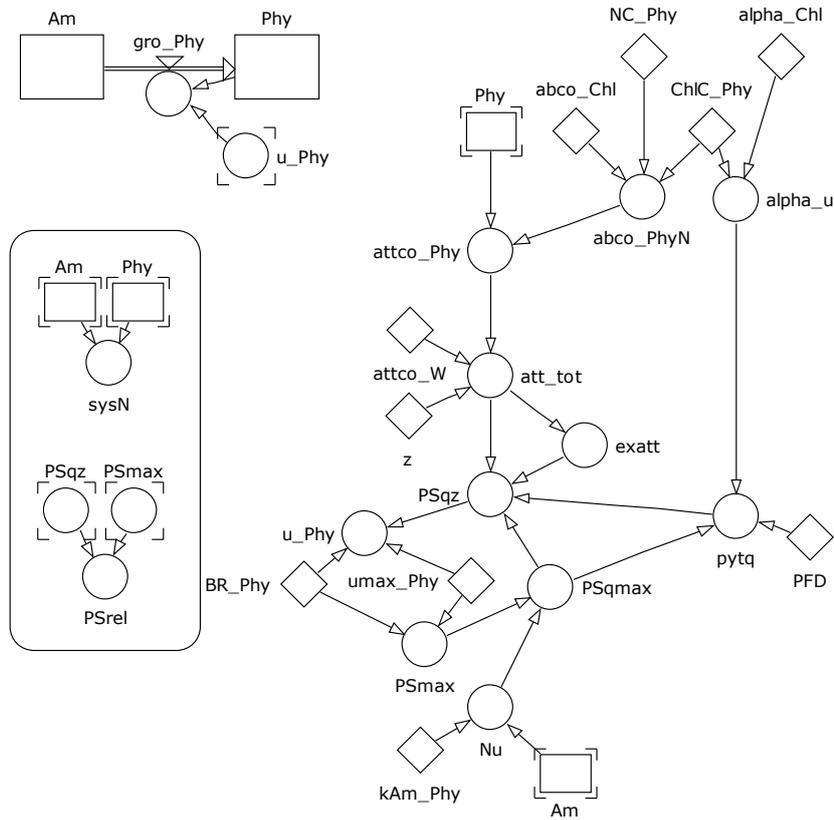


Fig. 8.2 Simple coupled nutrient-light limited phytoplankton growth model describing growth in a culture system of stated depth.

| Parameter | Type | Value | Unit | Description |
|------------------|------|--|---|---|
| <i>Am</i> | SV | 280 - <i>gro_Phy</i> | µgN L ⁻¹ | Ammonium-N concentration |
| <i>Phy</i> | SV | 1 + <i>gro_Phy</i> | µgN L ⁻¹ | Phytoplankton biomass-N concentration |
| <i>abco_ChI</i> | Con | 0.02 | m ² (mg ChI) ⁻¹ | Light absorbance coefficient for chlorophyll |
| <i>alpha_ChI</i> | Con | 7e-6 | (m ² g ⁻¹ ChI)*(gC µmol ⁻¹ photon) | Slope of ChI-specific PE curve |
| <i>attco_W</i> | Con | 0.05 | m ⁻¹ | Absorbance coefficient for growth medium (water) |
| <i>BR_Phy</i> | Con | 0.05 | dl | Scaler for basal respiration rate |
| <i>ChI_C_Phy</i> | Con | 0.06 | gChI (gC) ⁻¹ | Mass ratio content of chlorophyll:C in the phytoplankton |
| <i>kAm_Phy</i> | Con | 14 | µgN L ⁻¹ | Half saturation constant for <i>Am</i> limitation |
| <i>NC_Phy</i> | Con | 0.15 | gN (gC) ⁻¹ | Mass ratio content of N-biomass:C in the phytoplankton |
| <i>PFD</i> | Con | 500 | µmol photon m ⁻² s ⁻¹ | Surface irradiance (set here as a constant) |
| <i>umax_Phy</i> | Con | 0.693 | gN (gN) ⁻¹ d ⁻¹ | Phytoplankton maximum N-specific growth rate |
| <i>z</i> | Con | 10 | m | Water (optical) depth |
| <i>abco_PhyN</i> | Aux | $\frac{abco_ChI * ChI_C_Phy/NC_Phy}{}$ | m ² (mgN) ⁻¹ | Phytoplankton-N specific coefficient for light absorbance |
| <i>alpha_u</i> | Aux | $\alpha_ChI * ChI_C_Phy$ | (m ²)*(µmol ⁻¹ photon) | Specific slope of PE curve |
| <i>att_tot</i> | Aux | $z*(attco_W + attco_Phy)$ | dl | Total attenuation |
| <i>attco_Phy</i> | Aux | $abco_PhyN * Phy$ | m ⁻¹ | Attenuation coefficient to phytoplankton N-biomass |
| <i>exatt</i> | Aux | $EXP(-att_tot)$ | dl | Negative exponent of total attenuation |
| <i>gro_Phy</i> | Aux | $u_Phy * Phy$ | µgN L ⁻¹ d ⁻¹ | Phytoplankton population growth rate |
| <i>Nu</i> | Aux | $Am/(Am+kAm_Phy)$ | dl | Quotient for N-status |
| <i>PSmax</i> | Aux | $umax_Phy*(1+BR_Phy)$ | d ⁻¹ | Maximum gross photosynthetic rate required to enable $u_Phy=umax_Phy$ |
| <i>PSqmax</i> | Aux | $PSmax * Nu$ | d ⁻¹ | Maximum photosynthetic rate down-regulated by nutrient stress |
| <i>PSqz</i> | Aux | $\frac{pqmax*(LN(pytq+SQRT(1+pytq^2))-LN(pytq*exatt+SQRT(1+(pytq*exatt)^2)))}{att_tot}$ | d ⁻¹ | Phytoplankton N-specific growth rate |
| <i>PSrel</i> | Aux | $PSqz/PSmax$ | dl | Quotient for relative rate of PS |
| <i>pytq</i> | Aux | $(alpha_u * PFD * 24 * 60 * 60) / PSqmax$ | dl | Intermediate in depth-integrated photosynthesis rate |
| <i>sysN</i> | Aux | $Am + Phy$ | µgN L ⁻¹ | System N-balance |
| <i>u_Phy</i> | Aux | $PSqz - umax_Phy * BR_Phy$ | d ⁻¹ | Net growth rate |

Table 8.1 Main equations for coupled nutrient-light limited phytoplankton growth model. The value for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable. Note when checking units that µgN L⁻¹ equates numerically to mgN m⁻³.

8.6 Parameterising the Model

The model would be parameterised largely using the same approaches as for the phytoplankton model described in Chapter 4 (Section 4.8). Additionally, absorbance values could be determined by spectrophotometry, and the value of α estimated by conducting experiments to measure the PE curve (classically using ^{14}C or O_2 methodologies, though PAM-fluorometry based so-called “rapid-light-curves” could be used). To determine the basal respiration rate would require an O_2 methodology, such as using an oxygen electrode.

8.7 Operating the Model

Some example outputs are given in Fig. 8.3. Note the form of the population growth is now linear over much of the time, rather than being exponential over the period of nutrient availability (as it was using the model developed in Chapter 4, which did not consider light limitation). In this example output severe nutrient limitation (ca. $Nu < 0.5$) represents only a fraction of total nutrient+light limitation ($PSrel$) for much of the simulation; only with small values of z and low initial nutrient (and hence low biomass potential with little development of culture self-shading) is nutrient limitation the primary restrictor of growth throughout the simulation period.

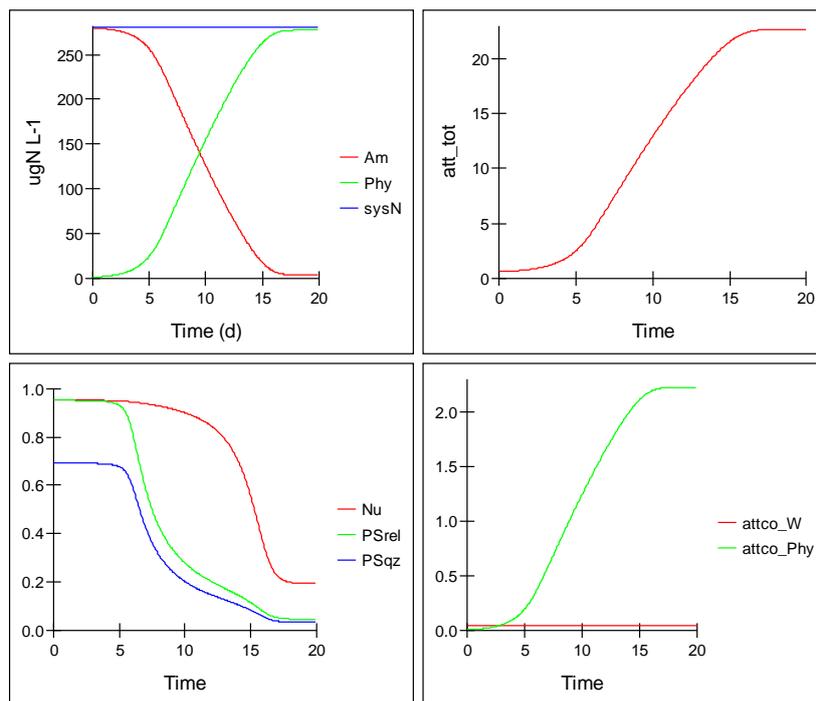


Fig. 8.3 Example model output for coupled nutrient-light limited phytoplankton growth model. Initial ammonium (Am) is set as $280 \mu\text{g N L}^{-1}$ ($=20 \mu\text{M}$), and mixing depth (z) at 10m. The model was run with Euler integration with a time-step of 0.0625 d.

8.8 Things to Explore

- i) Run the model with different irradiance (PFD), water depths (z), different nutrient loads (Am), and different water absorbance ($attco_W$). Note the conditions under which nutrient rather than light limits growth (see plot of Nu and $PSrel$ vs time in Fig. 8.3)
- ii) Couple the zooplankton model, the predator component, from Chapter 5 to this model. Assume that zooplankton add no significant light attenuation contribution. See how the predator-prey interaction affects the dynamics not just in consequence of the recycling of N, but because of the development and then removal of light-limitation as the phytoplankton biomass develops during growth and collapses during predation.
- iii) Couple the dilution components from Chapter 7 to either this model (as per (i)), or to that including the zooplankton (as per (ii)) and see how light-limitation affects the overall dynamics.

8.9 Caveats

While this model, and its predator-prey counterparts, represent a significant advance, there are two major caveats.

- The model assumes a fixed organism N:C. As we shall see in Chapter 15, this is not only a gross simplification but the implications of a variable N:C are profound for the dynamics of ecology via predator-prey interactions (Chapters 16 & 17). This forms the bedrock of Sterner & Elser's (2002) book on *Ecological Stoichiometry*.
- The model assumes that phytoplankton Chl:C is constant. It is not, but varies over a range of ca. 5 fold; the value used here is at the upper extreme of the range. The value of Chl:C affects the calculated attenuation and thus the level of self-shading affecting population dynamics, and will also affect the slope of the PE curve.

8.10 Where Next

To more completely describe the events considered here it is necessary to use a multi-element, variable stoichiometric model, in which C:N:Chl vary with nutrient and light. This is developed in several models in the literature (e.g., Flynn 2001, Flynn et al. 2001). However, light itself is such an important driver in plankton ecology that it is useful to consider some other options to enhance its description; this is considered in Chapter 9.

9. Describing Light

Terms and concepts introduced in this chapter- light units, astronomical light

9.1 Ecological Context

In most considerations of ecology, the subjects of primary production, photosynthesis, and thence light, soon come to the fore. This is absolutely true of plankton ecology in the sunlit photic zone, but it is also true when considering the commercial exploitation of microalgae (and indeed of macroalgae). In Chapter 8 we explored the issue of light limitation for production, and how this was exacerbated by self-shading of and by the growing phytoplankton population within the water column. The surface irradiance in that instance was set by a constant, *PFD*. Here we explore describing *PFD* as a variable. What follows are not models as such; they are bolt-ons to models that allow light to be described in different ways.

The description of astronomical light originated from a model provided by Mike Fasham (NOC, Southampton, UK), with modifications as given in the appendices of Kenny & Flynn (2015, 2016).

9.2 A Note of Warning Concerning Units of Irradiance

When configuring a model for light to best resemble a given situation, it is important to note that measuring light is non-trivial. For laboratory work, levels of irradiance are typically described using phrases such as “at the surface of the flask”; levels of *PFD* in the literature usually record values on the culture vessel face closest to the light source. Some researchers record light in the centre of a plain-water-filled vessel using a 4π sensor (this looks like a small white ball on a stick) to better account for light coming from all angles, and also being bounced around inside the vessel. In all instances there is the added issue of the spectral quality of light (a function of the light source, be it natural light, tungsten, fluorescent strip, LED etc.) and also of the calibration of the light sensor.

Coupled to the above is the subject of the action-spectrum of the phytoplankton photosystems, which acclimates to the light regime encountered by the organism itself. The action-spectrum describes the relationship between photosynthesis and light provided at each wavelength. As the organisms acclimate by making different pigment types to capture photons across the range of 400-700nm, the biochemistry of the phytoplankton themselves affect changes in *PFD* and the spectrum of residual light available to support the next period of photosynthesis.

Light can also be recorded in various different units, such as foot-candles, lux, lumens, *PFD*, and Wm^{-2} , which do not easily relate to each other – see Thimijan & Heins (1983) for information on conversion factors.

It is all very complicated, to put it mildly. More worryingly, many experimentalists and most models pay scant regard to the light regime at all, even at the most basic descriptive level.

9.3 Square-wave Light-Dark Cycles

The simplest way to control light, and that which accords with typical laboratory practice, is to literally switch light on or off for specific periods of time.

Assuming the simulation time is in days, then constants are required to define the light level when lights are “on” (PFD_on) and also the fraction of the day when lights are “on” ($frac_L$). Thus we have a new definition of PFD as:

$$PFD = IF (FRAC(TIME) < frac_L, PFD_on, 0) \quad \text{Eq.9.1}$$

This equation says that when the fraction of the simulation time (set by TIME) is less than $frac_L$, then the lights are switched on and $PFD = PFD_on$. Otherwise, the lights are off and $PFD=0$. The start of the light cycle thus aligns with the start of each simulation day.

If it was desired to arrange the period of light symmetrically around the day (i.e. around $FRAC(TIME) = 0.5$) then the definition of PFD becomes:

$$PFD = IF (FRAC(TIME + (0.5 + frac_L/2)) < frac_L, PFD_on, 0) \quad \text{Eq.9.2}$$

9.4 A Model for Astronomical Light

The following describes light according to the astronomical cycle as it changes over the year at a given latitude on Earth. Defining natural levels of irradiance carries several challenges, which include the following:

Unit for description – light has been described using many units and they are not readily transformable (see Thimijan & Heins 1983).

Cloud cover – the amount of light that enters the atmosphere and then passes through to the water surface is affected by the amount of cloud cover; this varies with geographic location, by the month, day, hour and indeed often by the minute. Because of the rapid acclimation to light by the human eye, we are typically unaware of how variable natural surface irradiance levels actually are.

Reflectance of the water surface – in waters that are smooth or have various levels of surface roughness (due to wind and tide), and depending on the angle of illumination, more or less of the light that penetrates through the cloud and reaches the water is then reflected.

In addition, of course the amount of light falling at a given location varies with the calendar date and time. The description below contains a switch that allows the date within the year to be fixed (e.g., to allow you to repeat March 1st for the whole simulation), or to increment the date as the simulation progresses. The form of the sub-model is given in Fig. 9.1, with the equations in Table 9.1.

Inputs to the model are the Julian date (JD ; in our context this is the date given as a number, where day 0 is 21st December of the period starting the simulation), the latitude (lat), and the index of cloud cover ($atmos_clar$). As the Earth moves around the sun so its declination angle changes (this is the angle at which the sun strikes the Earth’s surface at midday, shifting with the

9.6 Where Next

To more fully explore the commercial growth of phytoplankton consider using a variable stoichiometric model see Chapter 15. Also, see Kenny & Flynn (2016) for further discussions.

| Parameter | Type | Value | Unit | Description |
|--------------------|------|---|---|--|
| <i>atmos_clar</i> | Con | 0.55 | dl | corrects for atmospheric clarity (varies with lat, long & JD) |
| <i>con_fact</i> | Con | 4.57 | dl | converts W m ⁻² to PAR μmol m ⁻² s ⁻¹ for cloud-less sky with sun |
| <i>lat</i> | Con | 0-90 | ° | Latitude |
| <i>solar_const</i> | Con | 1368 | Wm ⁻² | solar constant irradiance (Wm ⁻² = J/m ² /s); maximum irradiance to Earth from the sun |
| <i>set_JD</i> | Con | {set for the day of interest} | d | required fixed date (see <i>sw_JD</i>) |
| <i>sw_JD</i> | Con | 0,1 | dl | switch; if 0 then date is fixed to <i>set_JD</i> ; if 1 then increment with TIME |
| <i>coszen</i> | Aux | MAX(SIN(<i>r_lat</i>)*SIN(<i>sol_deca</i>)+COS(<i>r_lat</i>)*COS(<i>sol_deca</i>)*COS(<i>r_hr</i>),0) | dl | cosine of zenith angle; positive values only accepted |
| <i>d_cal1</i> | Aux | -1*TAN(<i>r_lat</i>)*TAN(<i>sol_deca</i>) | dl | intermediate #1 in day length calculator |
| <i>d_cal2</i> | Aux | $d_cal1*(d_cal1>-1)*(d_cal1<=1)+-1*(d_cal1<=-1)+1*(d_cal1>1)$ | dl | intermediate #2 in day length calculator |
| <i>d_len</i> | Aux | (2*ARCCOS(<i>d_cal2</i>)*12/PI) | hr | day length at current Julian date |
| <i>d_len_frac</i> | Aux | <i>d_len</i> /24 | d | day length at current Julian date |
| <i>deg_1</i> | Aux | (<i>theta1</i> * 1.0<<deg/rad>>) | ° | angle the sun makes with the vertical (solar zenith angle) |
| <i>dusk</i> | Aux | (0.5+ <i>d_len_frac</i> /2) | d | time of dusk |
| <i>E_enter</i> | Aux | $1-(1.15E-06*deg_1^3 - 6.9134E-05*deg_1^2 + 0.001*deg_1 + 0.0187)$ | dl | proportion of light incident with the water surface that is just under the surface, accounting for reflectance |
| <i>frac_day</i> | Aux | FRAC(TIME) | dl | current time as fraction of day |
| <i>deg_hr</i> | Aux | ABS(12- <i>t24</i>)*15 | dl | degrees of hour angle away from noon (default 12:00) |
| <i>JD</i> | Aux | (<i>sw_JD</i> =1)*(365*(FRAC((TIME+10)/365)))+(sw_JD=0)* <i>set_JD</i> | d | Julian day; note the 10d offset (starting the year on 22 nd December) |
| <i>nat_PFD</i> | Aux | <i>Wm2_enter</i> * <i>con_fact</i> | μmol photon m ⁻² s ⁻¹ | PFD just under surface |
| <i>noon_coszen</i> | Aux | MAX(SIN(<i>r_lat</i>)*SIN(<i>sol_deca</i>)+COS(<i>r_lat</i>)*COS(<i>sol_deca</i>)*COS(0),0) | dl | value of <i>coszen</i> at noon (hence COS(0) at end of definition) |
| <i>noon_Wm2</i> | Aux | <i>solar_const</i> / <i>r_vec</i> / <i>r_vec</i> * <i>noon_coszen</i> | W m ⁻² | maximum irradiance (at noon) on this Julian date |
| <i>r_hr</i> | Aux | <i>deg_hr</i> *PI/180 | rad | hour angle radians |
| <i>r_lat</i> | Aux | <i>lat</i> *PI/180 | rad | latitude in radians |
| <i>r_vec</i> | Aux | $1/(1+0.033*COS(2*PI*JD*0.00274))^0.5$ | | Earth radius vector |
| <i>sol_deca</i> | Aux | $23.45*SIN(2*PI*(284+JD)*0.00274)*PI/180$ | rad | solar declination angle |
| <i>t24</i> | Aux | 24* <i>frac_day</i> | hrs | current time as fraction of day in hours |
| <i>theta1</i> | Aux | ARCCOS(<i>coszen</i>) | rad | angle the sun makes with the vertical (solar zenith angle) |
| <i>Wm2</i> | Aux | <i>solar_const</i> / <i>r_vec</i> / <i>r_vec</i> * <i>coszen</i> *(<i>coszen</i> >0) | W m ⁻² | irradiance at given hour and day; W m ⁻² [W = J s ⁻¹ ; i.e. J/m ² /s] |
| <i>Wm2_enter</i> | Aux | <i>Wm2</i> * <i>E_enter</i> * <i>atmos_clar</i> | W m ⁻² | light actually entering water (just under surface), accounting for reflectance |

Table 9.1 Description of astronomical light, including the effect of reflectance at the water surface

10. Pond Life

Terms and concepts introduced in this chapter- external data series; Q_{10} ; Arrhenius function

10.1 Ecological Context

One of the simplest operational structures for a real planktonic ecosystem is the humble pond. Ponds exist widely in terrestrial ecosystems as small, often transient, pools of water. They become inoculated with phytoplankton and zooplankton from cysts in the soil or sediment, blown in by the wind, or carried in by animals, such as water fowl. Ponds also exist as artificial structures in support of aquaculture or for the commercial production of microalgal biomass. And of course many contain fish, be they wild, ornamental or for food. Ponds are also important features of polar regions, developing as the ice melts.

In this chapter we will consider the pond as a habitat for growing plankton, subjected to inflows of water carrying nutrients, leakage, water evaporation and overflows. In some ways this chapter could be viewed as an extension to Chapter 7 on Dilutions, but there is a distinct difference in the core of the model structure. While hitherto we have considered state variables describing nutrient and biomass concentrations (e.g., as $\mu\text{gN L}^{-1}$), in the model described here the state variables describe absolute amounts; the concentrations themselves are thus auxiliaries. That is to say, we have state variables for the volume of water, the total mass of N in the pond as nutrient, and as plankton biomass.

In total this is a much larger and complex model than we have considered before. In consequence it is described in sub-models, each of which “talks” to other sub-models.

The equation are almost exclusively only provided in a linear format within the tables. You will need to cross reference the text commentary with the model schematic and tabulated information.

We will start by defining the pond itself with its entry and exit paths, and then introduce temperature changes in consequence of water exchange, evaporation and heat from the sun. Then we introduce the phytoplankton and zooplankton with growth affected by nutrients, light and also now by temperature.

You can make your *in silico* pond as large as you wish, into a lake if you wish. The caveat is that the model assumes a well-mixed water column.

The description of temperature and evaporation is developed from a sub-model originating from David Bowers (Bangor University, UK) used during joint research on growth of algal biomass in ponds.

10.2 The Pond and its Entries and Exits

We first need to define the dimensions of the pond. We will consider a simple pond, with one entry point of water, an overflow at a maximum capacity, a leakage to ground water, and also a

loss of water due to evaporation. The pond is visualised in Fig. 10.1; the components are described in Table 10.1.

Working around the sub-model we have the following components:

The pond itself, V_Pond , is described in terms of the volume of water it contains, as m^3 . It has a surface area, SA_Pond , and a depth (z_spill) measured from the deepest point to the bottom lip of a spillway from which water overflows. If your pond is not artificial, but has an irregular size, you could define surface area as a function of pond volume. This could make reference to real data from a pond; typically the surface area decreases rapidly as real ponds dry-out while this value will remain constant irrespective of depth for an artificial structure with vertical walls (as assumed here).

Water entry to the pond is defined by $inflow_Pond$, in this instance as an increasing rate that suddenly halts, rather akin to an increasing input from a storm event which then stops. You could replace this with a real data set describing a flow of $m^3 d^{-1}$; the flow could of course include that from rainfall directly upon the pond surface which you could add as a separate inflow.

Water enters the pond and increases its volume until the depth exceeds z_spill ; at that point water overflows down a spillway. The spillway has a width wid_spill . The actual depth of the water, z_Pond , can be lower than z_spill , or higher than it; the height above the lip (i.e., the depth of water flowing out of the spillway, which is the operational depth of the spillway) is zOp_spill . The rate of water flow from the spillway is then a function of the cross-sectional area of water in the spillway (XSA_spill) and acceleration due to gravity (g). You could introduce various spillways, as you wish. The sill in a real pond may be a deliberate construct (as assumed here) or it could amount to many overflow points around the pond periphery. You could build the pond in the form of a tidal-lagoon with the spillway actually a hole (or more likely a series of holes) of a set surface area at a certain depth which would differ depending on the relative height of water either side of the wall. In reality, the surface of the spillway would affect the flow of water due to turbulence; here we assume a simple smooth structure.

Water is also lost through seepage ($seep_Pond$) as a function of the porosity of the bottom ($SeepR$), the surface area and the water depth. Porosity of a real pond would typically be highly complex, related to cracks or changes in substrate (e.g., clay, rock types) in the pond base. The surface area would include the side walls, and the total area may be enlarged further depending on the bottom topography.

Finally, water is lost through evaporation ($evap_Pond$) as a function of the surface area and an evaporative rate related to temperature, humidity, and wind speed (see Section 10.3).

Note that there is no explicit description of the source or sinks of the water; hence the cloud symbols in Fig. 10.1.

The simulation is halted if the depth declines to a critical level, via $Stop_z$.

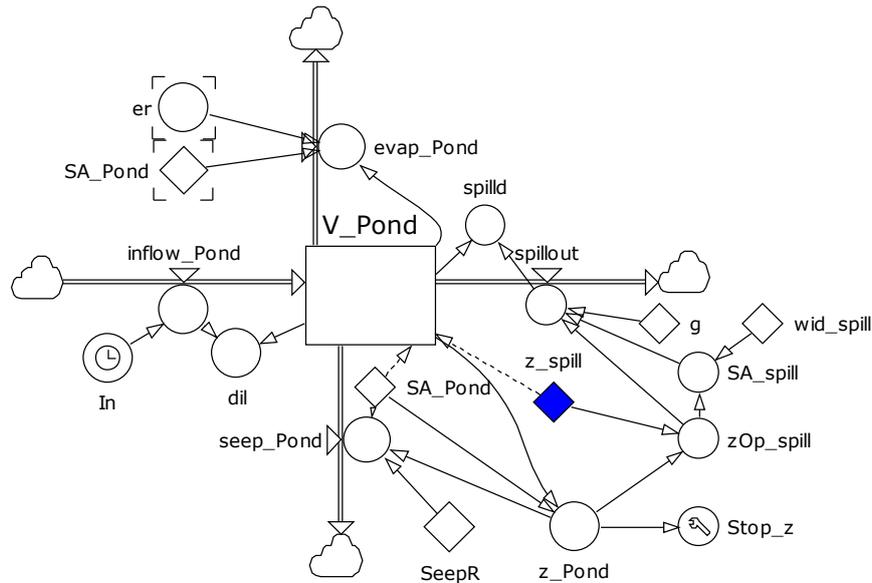


Fig. 10.1 The pond volume sub-model. See also Table 10.1.

| Variable | Type | Value | Unit | Description |
|-------------|------|--|--------------------------------|--|
| V_Pond | SV | $SA_Pond * z_spill$ <i>+ inflow_Pond</i> <i>- spillout</i> <i>- seep_Pond</i> <i>- evap_pond</i> | m ³ | Pond volume |
| g | Con | 9.81 | m s ⁻² | Acceleration due to gravity |
| SA_Pond | Con | 100 | m ² | Surface area of pond |
| SeepR | Con | 0.025 | d ⁻¹ | Seepage rate of water from the pond related to SA and per m of depth |
| wid_spill | Con | 0.05 | m | Width of spillway |
| z_spill | Con | 0.3 | m | Height of spill way lip above lowest point of pond |
| dil | Aux | $inflow_Pond / V_Pond$ | d ⁻¹ | Effective dilution rate of pond |
| er | Aux | {see Table 10.2} | m s ⁻¹ | Evaporation rate |
| evap_Pond | Aux | $IF(V_Pond > 0.1, (er * 60 * 60 * 24) * SA_Pond, 0)$ | m ³ d ⁻¹ | loss of water through evaporation |
| In | Aux | $IF(TIME < 10, 2 * TIME, 0) + 0.1$ | m ³ d ⁻¹ | Inflow of water |
| inflow_Pond | Aux | In | m ³ d ⁻¹ | Inflow of water |
| seep_Pond | Aux | $IF(z_Pond > 0, SeepR * SA_Pond * z_Pond, 0)$ | m ³ d ⁻¹ | Seepage loss of water |
| spilld | Aux | $spillout / V_Pond$ | d ⁻¹ | Specific dilution rate as would apply to phytoplankton |
| spillout | Aux | $60 * 60 * 24 * XSA_spill * (2 * g * zOp_spill)^{0.5}$ | m ³ d ⁻¹ | Loss of water through overflow through a spillway |
| Stop_z | Aux | $STOPIF(z_Pond < 0.01)$ | dl | Stop command to halt simulation when water attains a minimum depth |
| XSA_spill | Aux | $zOp_spill * wid_spill$ | m ² | Area of the mouth of the spillway |
| z_Pond | Aux | $IF(V_Pond > 0, V_Pond / SA_Pond, 0)$ | m | Depth of pond water |
| zOp_spill | Aux | $IF(z_Pond > z_spill, z_Pond - z_spill, 0)$ | m | Depth of water over spillway |

Table 10.1 Pond volume sub-model. See Fig. 10.1. dl dimensionless. The values for state variable are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

10.3 Water Temperature and Evaporation

Pond water temperature is altered by the temperature of the incoming water flows, and by heat exchange across the material that lines the pond; we will ignore the last mentioned as this transfer is usually slow. Temperature is also affected by the incident irradiance, the air temperature, wind and humidity (which collectively affect evaporation) and also by cloud cover which affects dark radiation of heat back into space (most notably at night with no cloud cover). Changes in pond water temperature (especially over the day-night, cycle) become increasingly apparent as the pond dries out because the residual water volume provides an ever decreasing buffer against temperature changes.

Temperature calculations can be complex; here we use a description of intermediate complexity. The extent to which you wish, or need, to build this sub-model depends greatly on the depth of the pond. Once the system becomes deeper than 1 m then changes in temperature due to heat exchange and evaporation become very slow. Furthermore, the required assumption of a homogenous mixed water layer becomes less easy to satisfy. If you have access to a data series to describe changes in the water temperature it would be more logical to replace the state variable T_{Pond} with an auxiliary describing the temperature. We consider using such external data in Section 10.4.

The sub-model structure is illustrated in Fig. 10.2, with equations in Table 10.2.

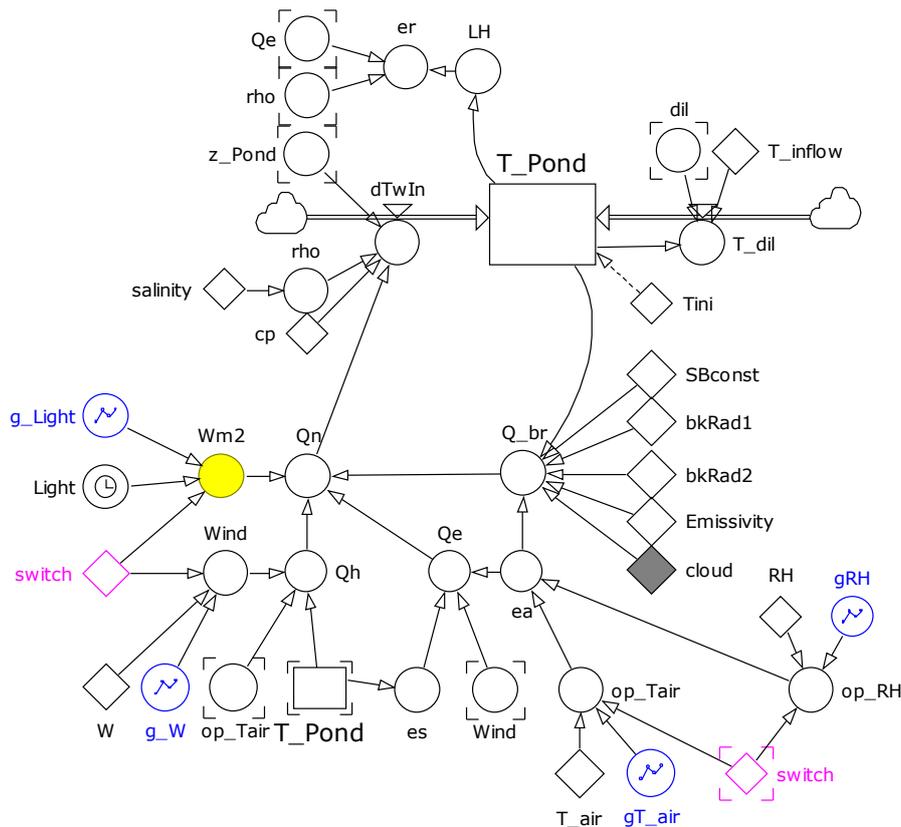


Fig. 10.2 The temperature sub-model. See also Table 10.2.

Let us work our way around the sub-model. The state variable describes the temperature of the pond water. There are two flows of heat into the system; both are indicated here as flows “in”, but it is important to note that (as always) that a negative flow “in” is the same as a flow “out”.

T_dil simply describes changes in T_pond as inflowing water mixes with the existing pond volume. The complex part, $dTwin$, is a mix of semi-empirical and physical descriptions accounting for the interactions of energy entering from sunlight ($Wm2$), temperature differences between the air (op_Tair) and T_Pond , backscatter of thermal energy to space (Q_br) which is affected by cloud cover, and heat loss associated with evaporation of water (Qe), a process affected by the relative humidity (op_RH) and op_Tair .

The rate of evaporation, er , is used to modify the volume of water in the pond (see Fig. 10.1; Table 10.1). The value of T_pond is used to alter the growth rates of the biological components; see Section 10.6.

There is scope for either using fixed values for controlling relative humidity, air temperature, light and wind speed, or you could describe these through reference to an external data set. This is considered further in Section 10.4, with selection between these options controlled by the constant *switch*.

{This space is intentionally blank; see next page for Table 10.2}

| Variable | Type | Value | Unit | Description |
|-------------------|------|---|----------------------------------|--|
| <i>T_Pond</i> | SV | <i>Tini</i> <i>+ dTwn</i> <i>+ T_dil</i> | °C | Temperature of pond water |
| <i>bkRad1</i> | Con | 0.05 | 1/mb ^{0.5} | Back radiation constant |
| <i>bkRad2</i> | Con | 0.35 | dl | Back radiation constant |
| <i>cloud</i> | Con | 2 | oktas | Cloud cover (0 to 8) |
| <i>cp</i> | Con | 4186 | J/kg°C | Specific heat of water |
| <i>Emissivity</i> | Con | 0.985 | dl | Emissivity of thermal radiation |
| <i>RH</i> | Con | 30 | % | Relative humidity |
| <i>salinity</i> | Con | 0 | dl | Salinity |
| <i>SBconst</i> | Con | 5.73E-08 | W/m ² /K ⁴ | Stefan-Boltzmann constant |
| <i>switch</i> | Con | 0 | 0 = fixed; 1 = data input | Switch between fixed or data input values |
| <i>T_air</i> | Con | 20 | °C | Air temperature |
| <i>T_inflow</i> | Con | 6 | °C | Inflow water temperature |
| <i>Tini</i> | Con | 10 | °C | Initial pond temperature |
| <i>W</i> | Con | 10 | m s ⁻¹ | Wind speed |
| <i>dil</i> | Aux | {see Table 10.1} | d ⁻¹ | Effective dilution rate of pond |
| <i>dTwn</i> | Aux | $(Qn/(cp*\rho*z_Pond))*60*60*24$ | °C d ⁻¹ | Rate of change of temperature due to heating and cooling |
| <i>ea</i> | Aux | $(op_RH/100)*6.11*10^{(7.5*op_Tair/(op_Tair+237))}$ | mb | Water vapour pressure in the atmosphere |
| <i>er</i> | Aux | $Qe/(LH*\rho)$ | m s ⁻¹ | Evaporation rate |
| <i>es</i> | Aux | $6.11*10^{(7.5*T_Pond/(T_Pond+237))}$ | mb | Saturated vapour pressure |
| <i>g_Light</i> | Aux | Data input | W m ⁻² | Light input data |
| <i>g_W</i> | Aux | Data input | m s ⁻¹ | Wind input data |
| <i>gRH</i> | Aux | Data input | % | Relative humidity data |
| <i>gT_air</i> | Aux | Data input | °C | Air temperature data |
| <i>LH</i> | Aux | $1000*(2500.8-2.36*T_Pond+0.0016*T_Pond^2-0.00006*T_Pond^3)$ | J kg ⁻¹ | Latent heat of water evaporation |
| <i>Light</i> | Aux | IF (FRAC(TIME)<0.5,300,0) | W m ⁻² | Light input |
| <i>Q_br</i> | Aux | $(1-0.1*cloud)*Emissivity*SBconst*(bkRad2-bkRad1*SQRT(ea))*(T_Pond+273)^4$ | W m ⁻² | Back radiation |
| <i>Qe</i> | Aux | $(3.8*(es-ea)*Wind)$ | W m ⁻² | Cooling evaporative heat flux |
| <i>Qh</i> | Aux | $2.5*(T_Pond-op_Tair)*Wind$ | W m ⁻² | Sensible heat flux from pond |
| <i>Qn</i> | Aux | $Wm2-(Q_br+Qe+Qh)$ | W m ⁻² | Net heat flux |
| <i>op_RH</i> | Aux | IF((switch=0), 1, 0)*RH+IF((switch=1), 1, 0)*gRH | % | Operational relative humidity |
| <i>rho</i> | Aux | $1000+salinity$ | kg m ⁻³ | Water density |
| <i>T_dil</i> | Aux | $(T_inflow-T_Pond)*dil$ | °C d ⁻¹ | Change in water temperature with incoming water |
| <i>op_Tair</i> | Aux | IF((switch=0), 1, 0)*T_air+IF((switch=1), 1, 0)*gT_air | °C | Operational air temperature |
| <i>Wind</i> | Aux | IF((switch=0), 1, 0)*W+IF((switch=1), 1, 0)*g_W | m s ⁻¹ | Operational wind speed |
| <i>Wm2</i> | Aux | IF((switch=0), 1, 0)*Light+IF((switch=1 AND g_Light>0), 1, 0)*g_Light | W m ⁻² | Light at the pond surface |
| <i>z_Pond</i> | Aux | {see table 10.1} | m | Depth of pond water |

Table 10.2 Temperature sub-model. See Fig. 10.2. dl dimensionless. The values for the state variable are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable. For “data input” see Section 10,4

10.4 Using External Data Series

As you will likely appreciate, external physical factors greatly affect ecology. While some of those factors work via direct involvement of the biological processes themselves (most obviously in our models via self-shading which decreases the available light for primary production; Chapter 8) other factors are sufficiently external that there is no bidirectional linkage that warrants explicit description in the simulations.

In Table 10.2 there are four such external, weather-related, drivers of the system. These can be controlled using the example data series given in Table 10.3.

| Day Time | Light (W m^{-2}) | Wind (m s^{-1}) | RH (%) | T air ($^{\circ}\text{C}$) |
|----------|-----------------------------|----------------------------|--------|------------------------------|
| 0.000 | 0 | 0 | 65 | 9 |
| 0.042 | 0 | 0 | 65 | 9 |
| 0.083 | 0 | 0 | 63 | 8 |
| 0.125 | 0 | 0 | 75 | 7.5 |
| 0.167 | 0 | 0.45 | 75 | 7 |
| 0.208 | 0 | 0 | 75 | 7 |
| 0.250 | 0 | 0 | 73 | 7 |
| 0.292 | 10 | 0 | 67 | 8 |
| 0.333 | 110 | 0 | 63 | 10 |
| 0.375 | 220 | 0 | 60 | 12 |
| 0.417 | 250 | 1.8 | 42 | 14 |
| 0.458 | 500 | 4.5 | 31 | 17.5 |
| 0.500 | 660 | 4.5 | 25 | 19 |
| 0.542 | 670 | 4.95 | 19 | 20 |
| 0.583 | 520 | 4.95 | 21 | 19 |
| 0.625 | 210 | 4.05 | 25 | 19 |
| 0.667 | 270 | 4.5 | 35 | 19 |
| 0.708 | 150 | 4.95 | 40 | 18 |
| 0.750 | 40 | 4.05 | 50 | 16 |
| 0.792 | 0 | 3.15 | 57 | 14 |
| 0.833 | 0 | 1.8 | 75 | 13 |
| 0.875 | 0 | 1.8 | 80 | 12 |
| 0.917 | 0 | 0 | 90 | 11 |
| 0.958 | 0 | 0 | 92 | 11 |
| 1.000 | 0 | 0 | 95 | 12 |

Table 10.3 Data series describing changes in light, wind speed, relative humidity and air temperature over a day. See also Fig. 10.3.

As can be seen from Fig. 10.3, these conditions are not constant, and to an extent they also interact with each other as the weather develops over the day. How you make your model interact with such external data series will depend on the platform that you employ. You may for example make your software platform interact directly with a spreadsheet containing the data during the simulation, or you may directly input the data series into the model code. Powersim Studio allows both options; the functions for direct entry via code looks like this for each of these variables:

g_Light=

```
GRAPHCURVE(FRAC(TIME),0,0.0416667,{0,0,0,0,0,0,0,10,110,220,250,500,660,670,520,210,270,150,40,0,0,0,0,0})
```

g_Wind=

```
GRAPHCURVE(FRAC(TIME),0,0.0416667,{0,0,0,0,0.45,0,0,0,0,1.8,4.5,4.5,4.95,4.95,4.05,4.5,4.95,4.05,3.15,1.8,1.8,0,0})
```

g_RH=

```
GRAPHCURVE(FRAC(TIME),0,0.0416667,{65,65,63,75,75,75,73,67,63,60,42,31,25,19,21,25,35,40,50,57,75,80,90,92,95})
```

g_air=

```
GRAPHCURVE(FRAC(TIME),0,0.0416667,{9,9,8,7.5,7,7,7,8,10,12,14,17.5,19,20,19,19,19,18,16,14,13,12,11,11,12})
```

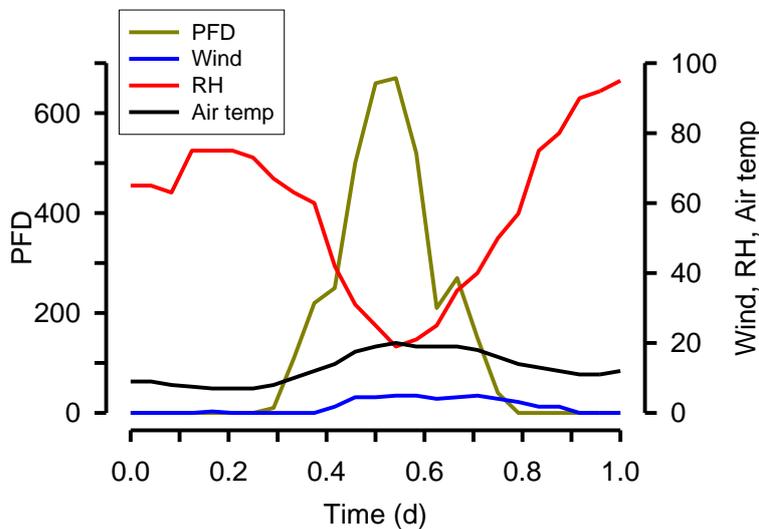


Fig. 10.3 Graphic representation of the data series in Table 10.3

The way that Powersim Studio reads these particular input functions (which report a daily cycle) is to repeat the usage of the data series at the end of the day, so the same cycles would be reproduced each day over the simulation period.

10.5 Nutrient Flows

We will consider only one nutrient here, naming it as dissolved inorganic N (N_{Pond} ; mgN). Note that this state variable describes an amount of nutrient in the pond; the nutrient concentration is given through reference to the pond volume, as N_{Pond}/V_{Pond} (DIN ; mgN m⁻³, converted here to μ M for use in the biology sub-models). At the start of the simulation we can set an initial amount of N. The amount of N in the pond changes depending on what is added via water inflow, removed with water via seepage and over the spillway, and removed or added by biological activity. Note that N is not removed with water evaporation; thus with all other entries and exits set at 0, DIN increases as evaporation decreases V_{Pond} while N_{Pond} remains constant.

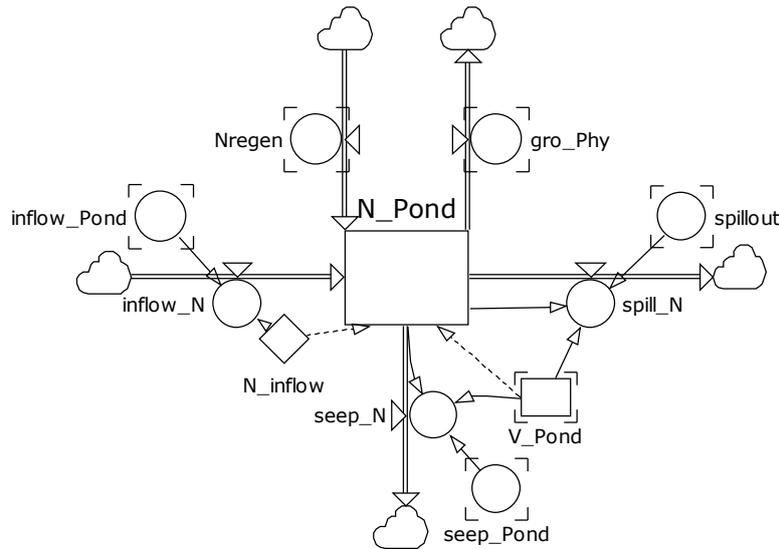


Fig. 10.4 The nutrient sub-model. See also Table 10.4.

| Variable | Type | Value | Unit | Description |
|--------------------|------|--|--------------------------------|--|
| <i>N_Pond</i> | SV | $V_Pond * N_inflow$ + <i>inflow_N</i> + <i>Nregen</i> - <i>seep_N</i> - <i>spill_N</i> - <i>gro_Phy</i> | mgN | Pond nutrient-N content |
| <i>V_Pond</i> | SV | {see Table 10.1} | m ³ | Pond volume |
| <i>N_inflow</i> | Con | 1400 | mgN m ⁻³ | Inflow concentration of N into pond |
| <i>gro_Phy</i> | Aux | {see Table 10.7} | mgN d ⁻¹ | Phytoplankton biomass growth |
| <i>inflow_N</i> | Aux | $inflow_Pond * N_inflow$ | mgN d ⁻¹ | Inflow of N into pond |
| <i>inflow_Pond</i> | Aux | {see Table 10.1} | m ³ d ⁻¹ | Inflow of water |
| <i>Nregen</i> | Aux | {see Table 10.7} | mgN d ⁻¹ | Regeneration of N by zooplankton as a consequence of grazing and respiration |
| <i>seep_N</i> | Aux | $N_Pond * seep_Pond / V_Pond$ | mgN d ⁻¹ | Loss of nutrient-N through seepage |
| <i>seep_Pond</i> | Aux | {see Table 10.1} | m ³ d ⁻¹ | Seepage loss of water |
| <i>spillout</i> | Aux | {see Table 10.1} | m ³ d ⁻¹ | Loss of water through overflow through a spillway |
| <i>spill_N</i> | Aux | $N_Pond * spillout / V_Pond$ | mgN d ⁻¹ | Loss of nutrient-N over the spillway |

Table 10.4 Temperature sub-model. See Fig. 10.4. dl dimensionless. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

The entries and exits of N concurrent with the flows of water described in the pond volume sub-model (Fig. 10.1; Table 10.1) are computed through reference to the flow rates and the concentration of N in the water. The concentration of N in the inflow (*N_inflow*) is considered constant though in reality it would vary with the rate and types of water inflow (such as decreasing with storm-water inflow, increasing seasonally if it was runoff from adjoining recently fertilized land). You could, for example, control this concentration, and indeed the rate of water inflow (*inflow_Pond*) from an external data series (see Section 10.4).

Fluxes of N due to biological activity are in support of phytoplankton growth (*gro_Phy*) and from N-regeneration (*N_regen*). These processes are described below (Section 10.8). But first we need to relate temperature to the rates of biological activity.

10.6 Temperature and Biological Rate Processes

Before describing the biological components, let us consider the changes required to the biological descriptions to involve temperature in the dynamics of ecology.

Hitherto we have assumed set maximum growth rates in our models. In reality, biochemical, and thence whole-organism biological processes are affected significantly by temperature. Temperature not only increases reaction rates, but it increases damage and thence turnover rates. In consequence the relationship between temperature and organism physiology is highly complex, and simple relationships are operable only over a narrow temperature span. All too easily temperature can increase to lethal levels, though in water the high specific heat capacity slows the rate of change. You will see when you run the model that if the pond is shallow enough, and if input weather conditions are conducive, then significant diel changes in *T_Pond* will develop. And these become exaggerated as evaporation makes the pond shallower.

Here we employ the simplest route to relate growth rates to temperature. As a rule of thumb, for a 10°C increase in temperature, biological rate processes double; this is often referred to as **Q₁₀=2**. This is typically described using the **Arrhenius function**. The Arrhenius function takes various forms (depending on applications), but the cut-down version used for biology is:

$$U_T = U_{ref} \cdot Q_{10}^{\left[\frac{(T-T_{ref})}{10}\right]} \quad \text{Eq.10.1}$$

Here, U_{ref} is the process rate at the reference temperature, T_{ref} . Q_{10} is the multiplier for changes in the rate per 10°C, and U_T is the process rate at temperature T . We will assume that our system operates within a range consistent with non-lethal temperatures and that this Q_{10} relationship holds throughout plausible simulations for our model.

There is one other assumption (simplification) we make here – we assume a single Q_{10} for each of the phytoplankton and zooplankton. In reality different components of physiology (e.g. photosynthesis vs respiration vs digestion) may be affected differently.

The sub-model is given in Fig. 10.5, with equations in Table 10.5. The driver for this sub-model is the pond temperature, reported by *T_Pond*. If you replace the temperature sub-model with an external data series describing water temperature (Section 10.4) than you need to link the Q_{10} calculations to those external data. Logic is that you replace the state variable *T_Pond* with an input auxiliary of the same name.

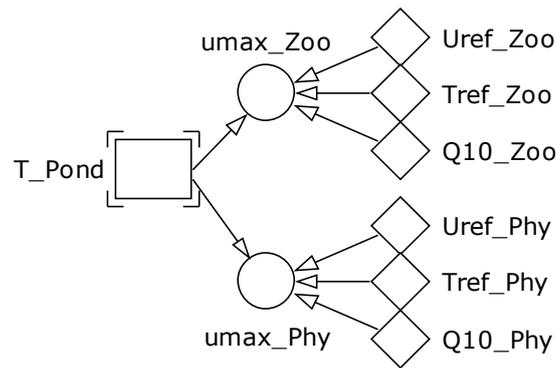


Fig. 10.5 The temperature – biological activity sub-model. See also Table 10.5.

| Variable | Type | Value | Unit | Description |
|-----------------|------|---|-----------------|--|
| <i>T_Pond</i> | SV | {see Table 10.2} | °C | Temperature of pond water |
| <i>Q10_Phy</i> | Con | 1.8 | dl | Phytoplankton Q ₁₀ |
| <i>Q10_Zoo</i> | Con | 2.2 | dl | Zooplankton Q ₁₀ |
| <i>Tref_Phy</i> | Con | 10 | °C | Reference temperature for phytoplankton growth |
| <i>Tref_Zoo</i> | Con | 10 | °C | Reference temperature for zooplankton growth |
| <i>Uref_Phy</i> | Con | 0.693 | d ⁻¹ | Phytoplankton maximum growth rate at reference T |
| <i>Uref_Zoo</i> | Con | 1.5 | d ⁻¹ | Zooplankton maximum growth rate at reference T |
| <i>umax_Phy</i> | Aux | $Uref_Phy * Q10_Phy^{((T_Pond - Tref_Phy)/10)}$ | d ⁻¹ | Temperature adjusted phytoplankton maximum growth rate |
| <i>umax_Zoo</i> | Aux | $Uref_Zoo * Q10_Zoo^{((T_Pond - Tref_Zoo)/10)}$ | d ⁻¹ | Temperature adjusted zooplankton maximum growth rate |

Table 10.5 The temperature – biological activity sub-model. See Fig. 10.5. dl dimensionless.

In the model described here we assume that the heterotrophic zooplankton are affected to a greater extent than are the phototrophic phytoplankton (i.e., *Q10_Zoo* > *Q10_Phy*).

10.7 Primary production

Phytoplankton growth is controlled by light and nutrient concentration. It is also affected by temperature, as described above, in Section 10.6; this gives us a value for the maximum growth rate (*umax_Phy*) that varies with water temperature (*T_Pond*). Other than this modification, the description of depth integrated photosynthesis related to the surface irradiance, pond depth and water attenuation, follows the approach described in Chapter 8. For completeness the sub-model and equations, with the above mentioned changes, are given here (Fig. 10.6; Table 10.6).

It should be noted that, as before, we assume homogenous mixing, though here the water depth is changing with alterations to inputs, leakage, overflow and evaporation.

Another feature of pond water is often a high load of humics (coloured dissolved organic matter, CDOM, mainly from higher plant decay) that significantly raises the water attenuation. That attenuation is affected by water flow off the land, by evaporation (removing water, but not CDOM), and by light which degrades CDOM over time. Here we will simply assume a fixed water attenuation value. You could control such changes through reference to an external data series informing the value of *attco_W*.

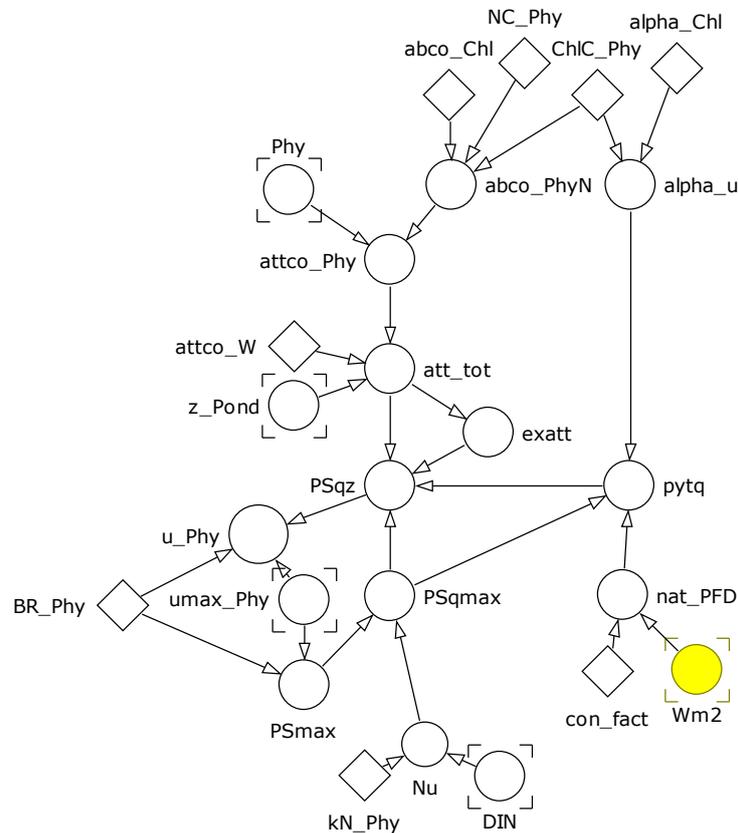


Fig. 10.6 Primary production sub-model. See also Table 10.6. The value of input light energy (Wm^2 ; yellow symbol) is input from an external data set, or from the model described in Chapter 9.

Note that because the basal respiration rate is referenced to the organism growth rate, both the photosynthetic rate and the respiration rate are informed by temperature-linked changes in activity. If desired (given suitable evidence), different values of Q_{10} could be used for different physiological processes.

The nutrient interaction makes reference to the concentration of inorganic N (*DIN*), which is itself a function of total inorganic N in the pond, and of the pond water volume.

| Variable | Type | Value | Unit | Description |
|------------------|------|---|---|--|
| <i>abco_ChI</i> | Con | 0.02 | m ² (mg ChI) ⁻¹ | Light absorbance coefficient for chlorophyll |
| <i>alpha_ChI</i> | Con | 7.00E-06 | (m ² g ⁻¹ chl.a)*(gC μmol ⁻¹ photon) | Slope of ChI-specific PE curve |
| <i>attco_W</i> | Con | 0.1 | m ⁻¹ | Absorbance coefficient for growth medium (water) |
| <i>BR_Phy</i> | Con | 0.1 | dl | Phytoplankton basal respiration as proportion of <i>umax_Phy</i> |
| <i>ChI_C_Phy</i> | Con | 0.06 | gChI (gC) ⁻¹ | Mass ratio content of chlorophyll:C in the phytoplankton |
| <i>con_fact</i> | Con | 4.57 | μmol s ⁻¹ W ⁻¹ | Correction factor to converts light as W/m ² to PAR |
| <i>kN_Phy</i> | Con | 14 | mg N m ⁻³ | Half saturation constant for <i>u_Phy</i> |
| <i>NC_Phy</i> | Con | 0.15 | gN (gC) ⁻¹ | Mass ratio content of N-biomass:C in the phytoplankton |
| <i>abco_PhyN</i> | Aux | <i>abco_ChI*ChI_C_Phy/NC_Phy</i> | m ² (mgN) ⁻¹ | Phytoplankton-N specific coefficient for light absorbance |
| <i>alpha_u</i> | Aux | <i>alpha_ChI*ChI_C_Phy</i> | (m ²)*(μmol ⁻¹ photon) | Specific slope of PE curve |
| <i>att_tot</i> | Aux | <i>z_Pond*(attco_W+attco_Phy)</i> | dl | Total attenuation |
| <i>attco_Phy</i> | Aux | <i>abco_PhyN*Phy</i> | m ⁻¹ | Attenuation coefficient to phytoplankton N-biomass |
| <i>DIN</i> | Aux | {see Table 10.7} | μM | Concentration of nutrient-N |
| <i>exatt</i> | Aux | EXP(- <i>att_tot</i>) | dl | Negative exponent of total attenuation |
| <i>nat_PFD</i> | Aux | <i>Wm2*con_fact</i> | μmoles m ⁻² s ⁻¹ | PFD at surface |
| <i>Phy</i> | Aux | {see Table 10.7} | μmolN L ⁻¹ | Phytoplankton biomass concentration |
| <i>PSmax</i> | Aux | <i>umax_Phy*(1+BR_Phy)</i> | d ⁻¹ | Maximum photosynthetic rate to balance <i>BR_Phy</i> to give <i>u_Phy=umax_Phy</i> |
| <i>Psqmax</i> | Aux | <i>Psmax*Nu</i> | d ⁻¹ | Maximum photosynthetic rate down-regulated in consequence of nutrient stress |
| <i>PSqz</i> | Aux | $\frac{Psqmax*(LN(pytq+SQRT(1+pytq^2))-LN(pytq*exatt+SQRT(1+(pytq*exatt)^2)))}{att_tot}$ | d ⁻¹ | Phytoplankton N-specific growth rate |
| <i>pytq</i> | Aux | $(alpha_u*nat_PFD*24*60*60)/Psqmax$ | d | Intermediate in depth-integrated photosynthesis rate |
| <i>umax_Phy</i> | Aux | {see Table 10.5} | d ⁻¹ | Temperature adjusted phytoplankton maximum growth rate |
| <i>u_Phy</i> | Aux | <i>PSqz-(umax_Phy*BR_Phy)</i> | d ⁻¹ | Phytoplankton growth rate |
| <i>Wm2</i> | Aux | {see Table 10.2} | W m ⁻² | Light at the pond surface |
| <i>z_Pond</i> | Aux | {see Table 10.1} | m | Depth of pond water |

Table 10.6 The primary production sub-model. See Fig. 10.6. dl dimensionless.

10.8 Ecology

And now to the ecological activity, which is described making use of a single phytoplankton and zooplankton function group approach as we have used before (Chapters 5 & 8). The sub-model is shown in Fig. 10.7 with equations in Table 10.7.

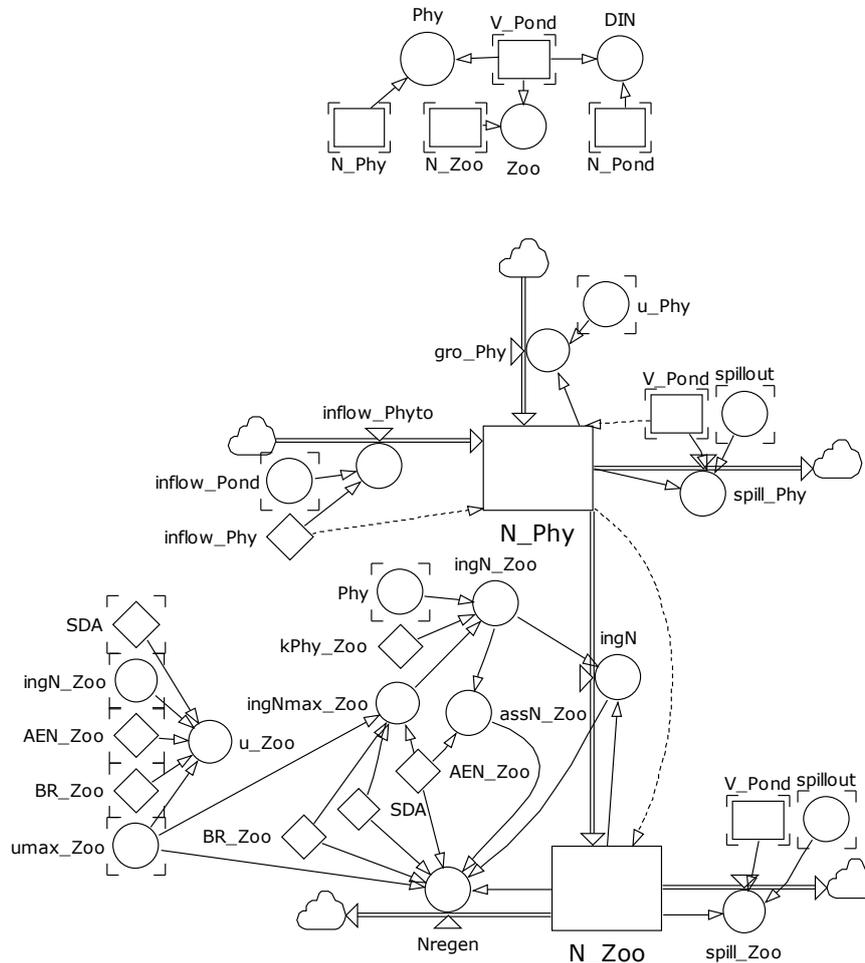


Fig. 10.7 Ecological activity sub-model. See also Table 10.7.

Note that the state variables for phytoplankton and zooplankton are given with units of mgN within the pond. Biological interactions are based upon concentrations of resources and not directly on these state variables; hence the derivation of concentrations DIN , Phy and Zoo through reference to V_Pond . Note that changes in water volume may occur without changes in the state variables for biomass and nutrients. Thus, as the pond dries due to evaporation, the concentrations of DIN , Phy and Zoo alter (increase) in the absence of any biological interactions.

In the model an inflow of phytoplankton is assumed; this may come from an up-stream pond or washed in from the land. Here that input is considered as a fixed concentration of phytoplankton, while in reality if there was a storm inflow of water the concentration of phytoplankton would be lower. As for other external linkages, you could drive this from an external data series.

| Variable | Type | Value | Unit | Description |
|---------------------|------|--|--------------------------------|--|
| <i>N_Phy</i> | SV | $inflow_Phy * V_Pond$ <i>+gro_Phy</i> <i>+inflow_Phyto</i> <i>-ing_N</i> <i>-spill_Phy</i> | mgN | Phytoplankton biomass |
| <i>N_Zoo</i> | SV | N_Phy <i>+ing_N</i> <i>-N_regen</i> <i>-spill_Zoo</i> | mgN | Zooplankton N-biomass |
| <i>V_Pond</i> | SV | {see Table 10.1} | m ³ | Pond volume |
| <i>AEN_Zoo</i> | Con | 0.6 | dl | Assimilation efficiency |
| <i>BR_Zoo</i> | Con | 0.2 | dl | Zooplankton basal respiration rate proportioned to <i>umax_Zoo</i> |
| <i>inflow_Phy</i> | Con | 10*14 | mgN m ⁻³ | Concentration of incoming phytoplankton biomass |
| <i>kPhy_Zoo</i> | Con | 5*14 | mgN m ⁻³ | Half saturation constant for zooplankton predation on phytoplankton |
| <i>SDA</i> | Con | 0.3 | dl | Specific Dynamic Action |
| <i>assN_Zoo</i> | Aux | $ingN_Zoo * AEN_Zoo$ | d ⁻¹ | Assimilation rate |
| <i>DIN</i> | Aux | $(N_Pond / V_Pond) / 14$ | μM | Concentration of nutrient-N |
| <i>gro_Phy</i> | Aux | $N_Phy * u_Phy$ | mgN d ⁻¹ | Phytoplankton biomass growth |
| <i>inflow_Phyto</i> | Aux | $inflow_Phy * inflow_Pond$ | mgN d ⁻¹ | Incoming phytoplankton; this also serves to inoculate the system |
| <i>inflow_Pond</i> | Aux | {see Table 10.1} | m ³ d ⁻¹ | Inflow of water |
| <i>ingN</i> | Aux | $N_Zoo * ingN_Zoo$ | mgN d ⁻¹ | Loss of phytoplankton through ingestion by zooplankton |
| <i>ingN_Zoo</i> | Aux | $ingNmax_Zoo * Phy / (Phy + kPhy_Zoo)$ | d ⁻¹ | Ingestion rate of phytoplankton |
| <i>ingNmax_Zoo</i> | Aux | $(umax_Zoo * (1 + BR_Zoo)) / (AEN_Zoo * (1 - SDA))$ | d ⁻¹ | Maximum ingestion rate, allowing <i>u_Zoo</i> = <i>umax_Zoo</i> under optimal conditions |
| <i>Nregen</i> | Aux | $N_Zoo * (umax_Zoo * BR_Zoo) + assN_Zoo * SDA + ingN * (1 - AEN_Zoo)$ | mgN d ⁻¹ | Regeneration of N by zooplankton as a consequence of grazing and respiration |
| <i>Nu</i> | Aux | $DIN / (DIN + kN_Phy)$ | dl | Index of N-limitation for phytoplankton growth |
| <i>Phy</i> | Aux | $(N_Phy / V_Pond) / 14$ | μmol N L ⁻¹ | Phytoplankton biomass concentration |
| <i>spillout</i> | Aux | {see Table 10.1} | m ³ d ⁻¹ | Loss of water through overflow through a spillway |
| <i>spill_Phy</i> | Aux | $N_Phy * spillout / V_Pond$ | mgN d ⁻¹ | Loss of phytoplankton biomass over the spillway |
| <i>spill_Zoo</i> | Aux | $N_Zoo * spillout / V_Pond$ | mgN d ⁻¹ | Loss of zooplankton biomass over the spillway |
| <i>u_Phy</i> | Aux | {see Table 10.6} | d ⁻¹ | Phytoplankton growth rate |
| <i>u_Zoo</i> | Aux | $ingN_Zoo * AEN_Zoo * (1 - SDA) - (umax_Zoo * BR_Zoo)$ | d ⁻¹ | Zooplankton growth rate |
| <i>Zoo</i> | Aux | $(N_Zoo / V_Pond) / 14$ | μmol N L ⁻¹ | Zooplankton biomass concentration |

Table 10.7 The biological activity sub-model. See Fig. 10.7. dl dimensionless. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

There is no assumed input of zooplankton with the inflowing water to the pond, though you could of course introduce one.

The zooplankton description is similar to that we have used before (Chapter 5), making prey ingestion a function of Phy through reference to half saturation constant $kPhy_Zoo$. Losses from zooplankton relate to assimilation efficiency (AE) and respiration associated with basal respiration (BR_Zoo) and SDA . As before, we assume an instantaneous regeneration of voided N in a form suitable for the support of primary production. In reality, losses with respiration would indeed be suitable (released as ammonium), but the faeces voided associated with $(1-AE)$ would sink (some may be lost via the overflow) and degrade slowly.

The trophic web (just a simple chain) is far simpler that would exist in anything other than an artificial pond. In a real pond the presence of fish to control zooplankton is commonly a critical determinant of the ecology. You could explicitly introduce additional zooplankton groups to graze on Zoo , or you could “cheat” and use what is termed a closure function (see Chapter 11).

10.9 Parameterising the Model

The overwhelming controlling factors in this model are physical. The pond size, depth, the descriptions of input, seepage and spillway are important factors. However, perhaps more important is the description of the climatic conditions of light, air temperature, wind, relative humidity and cloud cover. As described above, these climatic conditions can be described as simple fixed values, and for light as a square-wave, situations that would never occur in nature. Alternatively, many of the climatic processes interrelate over the day-night period (Fig. 10.3), and of course typically they vary day by day as well. Just repeating these each day introduces a significant dynamic, especially if the cloud cover is altered as well; here we assume that value is constant ($cloud; = 2$ oktas).

In addition to the physics, there are the usual biological components which require parameterisation as we have considered previously, in Chapters 4, 5, & 8.

10.10 Operating the Model

The model as described was operated with Euler integration with a step size of 0.015625 d, though you will need to undertake the usual checks, especially if you introduce different growth rates and climatic forcings.

Be particularly careful if the pond volume (V_Pond) approaches 0. Also note that certain combinations of climatic variables can result in the pond temperature (T_Pond) dipping to below 0; the model is not constructed to correctly describe such a transition physically, and of course certainly not biologically! Accordingly, you may wish to introduce some controls to stop the simulation should V_Pond and T_Pond attain certain values; there is already such a control in the pond volume sub-model.

Two example outputs are given, one with fixed physical forcings (Fig. 10.8), the other making reference to external data (Fig. 10.9).

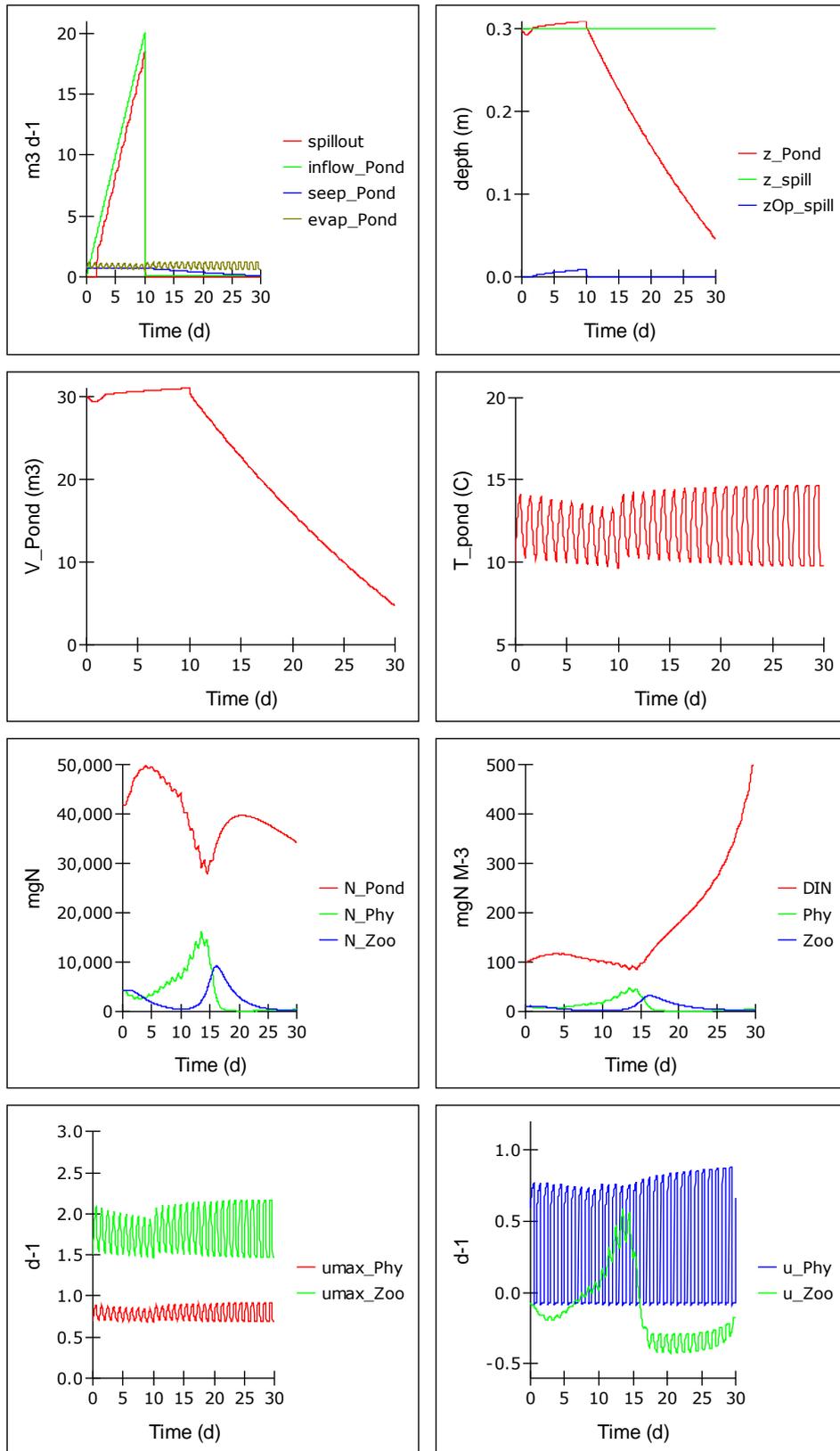


Fig.10.8 Model run using fixed external weather conditions.

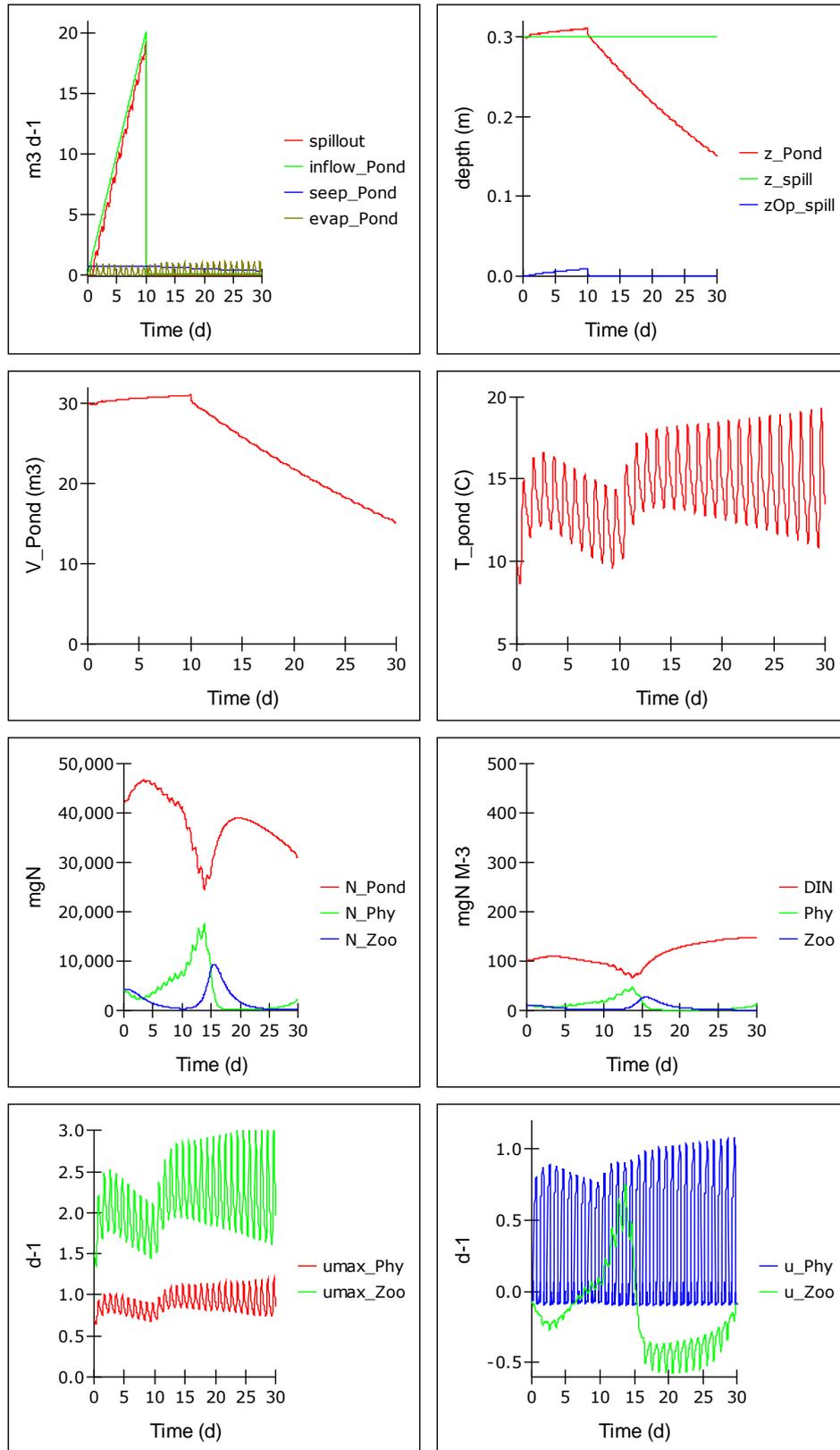


Fig.10.9 Model run using external weather conditions controlled by a repeating daily data series.

10.11 Things to Explore

There are very many opportunities for playing with this model, and likewise much scope for developing the model further. Below are some suggestions, most of which could be merged to provide further scope.

- i) Add a closure function (Chapter 11), or indeed an explicit description of a higher trophic level, to see what happens if zooplankton growth is controlled. From this you will see why ponds are so often green; if the zooplankton are grazed out by fish, then the phytoplankton grow uncontrolled. In real ponds, controlling phytoplankton is a major challenge, best achieved by limiting nutrient input. Pond depth also affects this interaction.
- ii) Introduce a coupled input series describing water and nutrient inflows, together with climate. You may be able to configure your pond against a real system, driving it with real climate data, with additional run-offs from adjoining land during storm events, or similar.
- iii) Modify the pond so that it represents a microalgal biotechnology or aquaculture bioreactor. Here the depth (z) will be ca. 0.2 – 0.3 m, and input and output will operate akin to a chemostat (Chapter 7). The impact of climate changes, as day-to-day weather, will affect productivity and hence your profit margins. Clear skies (lower value of $okta$ in *cloud*) promote higher photosynthetic rates, but will also induce a stronger diel temperature effect. The cold at night is beneficial as it restricts night-time respiration. However, if the cold takes some time to take off in the daylight then production is lowered.
- iv) Modify your pond so that it resembles a tidal lagoon. To do this replace the spillway area with an area describing the lagoon outflows; these are typically at some depth below the low tide level. You will need to describe what amounts to an adjoining “pond” (i.e., the ocean!) with its water height driven by a description of the tides; this could be done with reference to an external data series. The flows in and out will relate to the surface area of the holes, and to the operational depth difference between water either side of the lagoon wall.

10.12 Caveats

Most of the caveats have already been described above, or in Chapters 4, 5, & 8. The description of the physics of the system themselves represent gross simplifications; in a real settings there are many local climatic factors to take into account. Porosity of the bed of the pond, alone, can contribute significantly to errors in description of the system.

For the biological components, the absence of a description of the benthic processes, of the accumulation of detritus that over time results in the infilling of the pond, would typically be a major omission. There is also the omission of gas concentrations. The concentration of CO_2 , diffusing in from the atmosphere, being consumed by photosynthesis and released by respiration, can limit primary production, and also alter pH significantly (as can the nature of the water coming into the pond, as acid rain, for example). Oxygen concentrations can be super-saturating on warm bright days with high primary production, or conversely limiting during the night time if the community respiration is high enough. However, in a shallow well mixed system these factors may not be of such concern.

10.12 Where Next

In Chapters 15, 16 & 17 we consider variable stoichiometry and how that impacts the plankton trophic dynamics.

11. Closure

Terms and concepts introduced in this chapter- closure term, switch functions

11.1 Ecological Context –Handling Higher Trophic Levels

No model can ever describe everything; there have to be boundaries of in terms of physics, chemistry, biology, and of course time. So how do you handle these boundaries, and specifically here, how do you handle the upper most trophic level in an ecosystem model?

If you are modelling the changes in the volume of a lake then you do not need to simulate, in a consequence of the lake filling through rainfall, that the amount of moisture in the air must decrease. Neither will you likely need to simulate changes in the volume of the oceans as the lake water drains into the sea.

In models of food webs it is likewise often necessary to limit the detail at the lowest and uppermost reaches of the food web. It is rare that microbial communities are described in any detail, so that nutrient regeneration is treated rather as a black-box of organics entering and inorganics flowing out; this is the route we used in Chapters 5 and 10. The upper extremes of food webs contain top predators; these organisms (for aquatic systems, larger fish, whales, sharks, etc.) are often enigmatic and feature strongly in perceptions of importance. However, in reality they are often responsible for very little of the biomass and energy flows through food webs, while their activity is often also only occasional, being linked to movement of these animals between feeding areas. This is not to say that the activity of these higher trophic levels is not of importance in structuring the system, so somehow we need to include their activity. However, rather than describe their activity explicitly, we can describe it implicitly using a function called a **closure term**.

11.2 Closure Terms

A closure term is applied to control the extent of population growth of the uppermost trophic level which is described (i.e., for which a state variable is present). The term describes an implicit activity of the trophic level and of other factors such as disease above that which we describe explicitly. We have actually already used a closure term, within the L-V model in Chapter 6; there it constrained the population of the predator population that was described, although the same function in a systems ecology context would have included other loss terms, describing respiration and/or nutrient regeneration.

Closure terms can take various forms, but typically they are either linear or power functions of the population size of the last explicitly described group. What does that mean? Let us consider the simple model as we developed in Chapter 5 (reproduced here as Fig. 11.1).

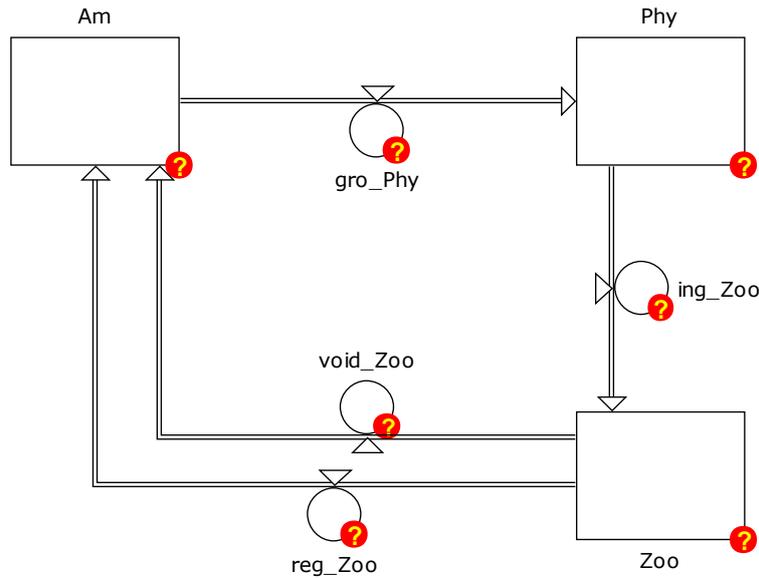


Fig 11.1 Conceptual predator-prey model from Chapter 5.

Here the system is closed, as may be expected in a flask system. Note also, as mentioned above, that there is an implicit involvement of a microbial community that is assumed to rapidly degrade voided material (faeces; $voidN_{Zoo}$) into ammonium (Am).

What we do not have is a predator controlling the growth of Zoo . Thus, if we start this system with a very high value of Am , in reality we may expect the dynamics to not be controlled by nutrient availability but by some other event. That event could be cannibalism by Zoo upon itself; such events are not uncommon in crowded communities of predators and its description here would still produce a model that is explicitly constrained. Alternatively (or additionally) the event could be controlled by some other density-dependant process linked to Zoo , such as disease or the activity of a higher predator; collectively these are the processes described by a closure term.

What we need is another flow of material out from Zoo that is a function of the size of Zoo (i.e., it is density dependant). Let us call that term $death_{Zoo}$ and define it as:

$$death_{Zoo} = death * Zoo \quad \text{Eq.11.1}$$

Or for a square-power version by:

$$death_{Zoo} = death * Zoo^2 \quad \text{Eq.11.2}$$

In general terms we can use this:

$$death_{Zoo} = K_{close} * (Zoo^{H_{close}}) \quad \text{Eq.11.3}$$

Here, K_{close} and H_{close} are constants controlling the closure event.

In all instances it is worth noting that there is no upper limit to the rate of loss. It is also noteworthy that we are not even defining the cause of death, only that we assume it to be density

dependant. In reality there are likely to be several processes acting simultaneously, if not in consort (consider a decay process mediated by various detritivores and microbes, for example).

We now need to decide what happens to this material, to the corpses. There are two obvious fates, though they are clearly not mutually exclusive.

1. The material flux described by *death_Zoo* could just be recycled in exactly the same way as material that is voided from *Zoo*, as described by *void_Zoo*; that is we assume that *death_Zoo* flows directly back to *Am*, making use of the same implicit microbial community we assumed to be acting on *void_Zoo*.
2. The material could be lost from the system. We could have a planktonic system from which corpses would sink out so that the proceeds of degradation are not available to support the continuing activity of the processes we have explicitly described. In reality, some of that material could be buried and released over geological time spans. On the other hand, it could be recycled in the depths, and come back into the system we have explicitly described as an entry of new nutrients into *Am*, driven by a physical process such as an upwelling at some time in the future. Incidentally, the latter is akin to considering a slow (rather than instantaneous) regeneration of *Am* from *void_Zoo*.

Let us now implement these alternatives within a structure that is flexible, so we can explore the implications of different options.

11.3 Building Flexibility into Models

As you will have realised by now, building and testing models can be non-trivial. In many instances a common core model can be used to support several activities, with alternate components switched in or out. In some instances this can be achieved simply by setting rate constants or initial state variable values as zero (or to prevent a “division by zero” error, by setting a very small value, such as $1e-100$). In other instances an explicit **switch function** can be used to implement different blocks of code. We have used such approaches earlier in this book (e.g., Chapter 10).

Switches are simply constants that take values such as 0 or 1 (off or on), or perhaps other values to configure more complex alternative structures.

11.4 The Model

We use as the base the model described in Fig. 5.3 and Table 5.1. To this we make the changes indicated in Table 11.1 so the structure now appears as in Fig. 11.2.

If it was desired to simulate the complete loss of material as corpses (the extreme form of option (2), Section 11.2, above), then *rate_decay* would be set as 0, and the state variable *Corpse* would accumulate the biomass that leaves the system. If *rate_decay* is set as 1 then the corpses spontaneously decay, as we assumed to be the fate of the voided matter in Chapter 5.

The switch, *sw_close*, controls whether the closure term operates (*sw_close* = 1) or not (*sw_close* = 0).

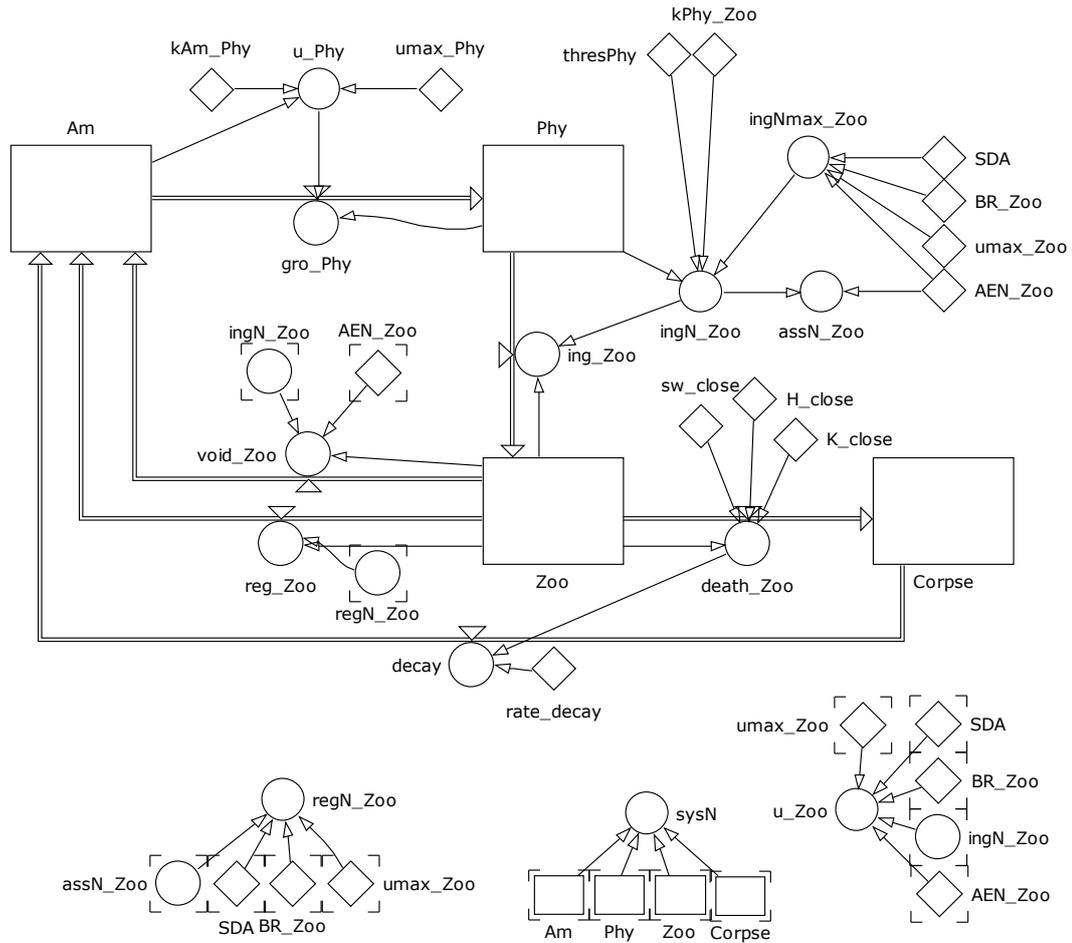


Fig 11.2 The complete model as per Table 5.1 with additions and updates in Table 11.1.

| Variable | Type | Value | Unit | Description |
|------------|------|--|-------------------------------------|--|
| Corpse | SV | 0 +death_Zoo -decay | $\mu\text{gN L}^{-1}$ | zooplankton corpse |
| H_close | Con | 2 | dl | power term for closure |
| K_close | Con | 0.01 | d^{-1} | constant term for closure |
| rate_decay | Con | 0.6 | dl | proportion of zoo_death decaying to Am (value between 0 and 1) |
| sw_close | Con | 1 | dl | switch to enact closure; 0 off, 1 on |
| decay | Aux | $\text{death_Zoo} * \text{rate_decay}$ | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | decay rate of corpse |
| sysN | Aux | $\text{Am} + \text{Phy} + \text{Zoo} + \text{Corpse}$ | $\mu\text{gN L}^{-1}$ | (revised) system |
| death_Zoo | Aux | $\text{IF}((\text{sw_close}=1), 1, 0) * \text{K_close} * (\text{Zoo}^{\text{H_close}})$ | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | closure term for death |

Table 11.1 Additions and updates to equations given in Table 5.1 to include closure.

11.5 Parameterising the Model

Closure is not something that you can simply measure. As it is a function of so many potential interactions, the values of variables controlling both closure and the description of the fate of the material removed by closure are often decided through trial and error. Or they may be determined more systematically by employing some form of tuning or optimisation approach (Chapter 14).

See Chapters 4 and 5 for other details on parameterising this model.

11.6 Operating the Model

The outputs shown in Figs. 11.3, 11.4 and 11.5 show the impacts of not only closure but what happens with differences in the fate of the *Zoo* removed by closure.

Fig. 11.3 is a longer term simulation akin to Fig. 5.4, with no closure term enacted, with a repeat predator-prey cycle developing rapidly. There are no corpses.

In Fig. 11.4, closure is enacted with the rate of decay at 60% of that of the death rate. *Corpse* accumulates, and indeed an increasing amount of *sysN* becomes locked out of the main system in consequence. It is apparent that the system is slowly approaching a dynamic equilibrium.

Fig. 11.5 also has closure enacted, so again there is a death term applied to *Zoo*, but this time we assume simultaneous remineralisation of *Corpse*, so there is no accumulation of N within that state variable. This gives quite different dynamics to that shown in Fig. 11.3, although neither show any *Corpse*. This demonstrates, amongst other things, how an indiscriminate hidden addition to a model can have profound impacts upon the dynamics. In this instance, not only are the dynamics of the closure of critical importance, but so is that associated with remineralisation through the detritivore and bacterial “black box”.

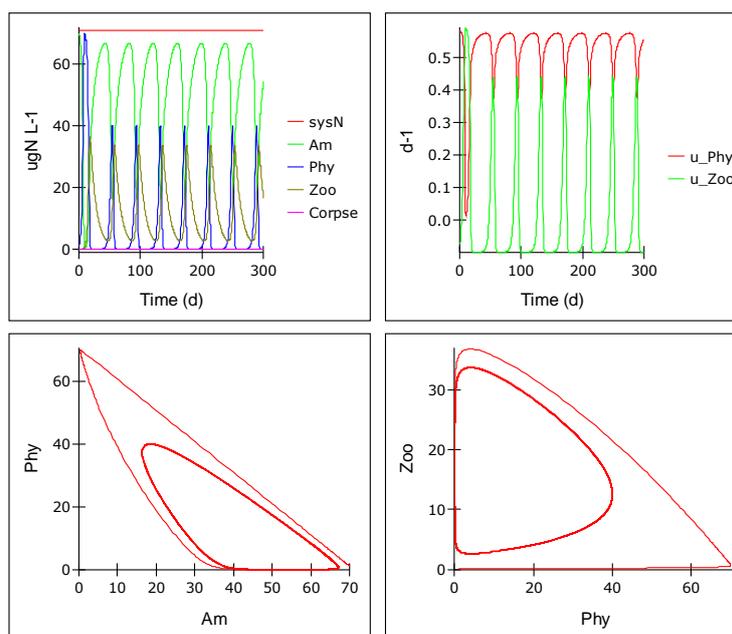


Fig. 11.3 Example model output without closure enacted.

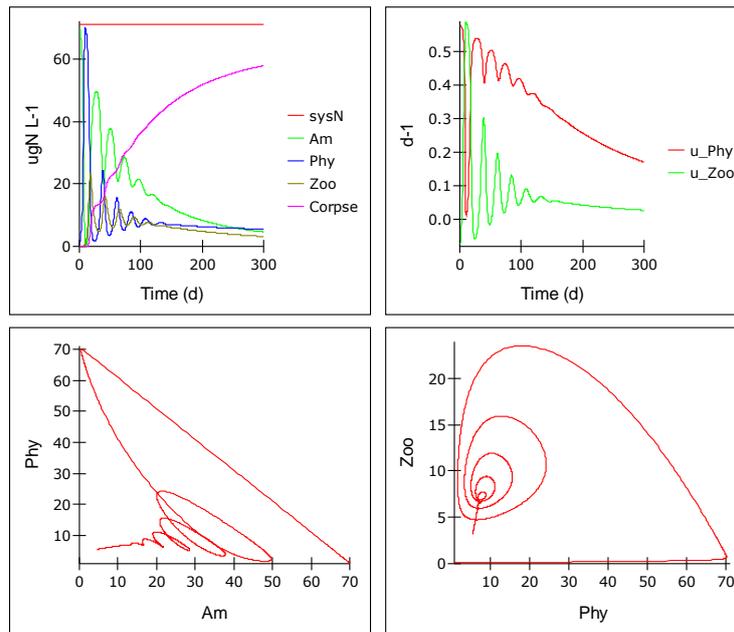


Fig. 11.4 As Fig. 11.3, by now with closure enacted (i.e., $sw_close = 1$), and $rate_decay = 0.6$. *Corpses* now accumulate.

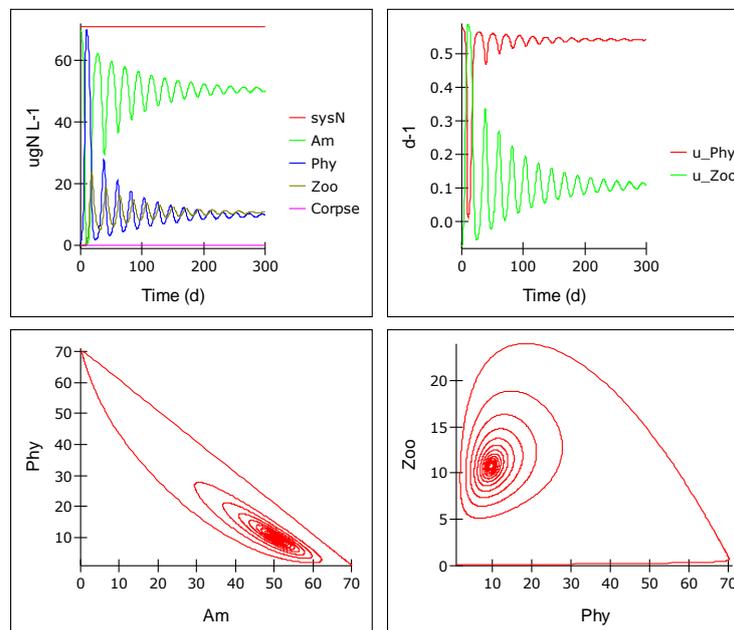


Fig. 11.5 As Fig. 11.4, with closure enacted (i.e., $sw_close = 1$), but now with $rate_decay = 1$. Here *Corpses* do not accumulate; through just reference to the existence of state variables with values >0 (i.e., *Am*, *Phy*, *Zoo*), this system appears similar in structure to that in Fig. 11.3 (i.e., no *Corpse*), but the dynamics are very different. Note that the lower panels show convergence to attractor points, while the analogous plots in Fig. 11.3 show convergence to attractor basins (See Section 2.11).

11.7 Things to Explore

- i) Alter the values controlling the closure function (H_close , K_close), noting that you can switch the function off or on simply by altering the value of sw_close from 0 (off) to 1 (on).
- ii) What happens if you commence the simulations with different initial values of Am and deploy different values of $rate_decay$? Note that if $rate_decay = 0$ then all the material flowing from $death_Zoo$ goes to *Corpse* and stays there; while $sysN$ will remain constant (proving that you have not made an error in the logic or maths!), the amount of material in the active system (i.e. $Am+Phy+Zoo$) decreases. As that process develops so the dynamics of the predator-prey interaction will change.
- iii) See what happens if you direct $void_Zoo$ to *Corpses*, so that faecal material degrades slowly and not spontaneously.
- iv) The rate of decay (remineralisation) of *Corpse* described here is related to the rate of death. You could, in contrast, make the rate of decay a type II (e.g., rectangular hyperbolic) function of the value of *Corpse*. To do that you need to introduce a maximum rate of decay and a half saturation constant. Think about this though; do you need to explicitly describe the biomass of the organisms mediating the decay processes? And what mediates the remineralisation of *Corpse* – should that also be a type II function, and if so, to what should it be related? You could also deploy a pipeline delay function (Section 2.3, “Flows”).

11.8 Caveats

The whole subject of closure is one upon which many have worked. Closure is rather a blunt instrument. For plankton systems, the vast bulk of death is attributed to events within the planktonic community itself. Most of “closure” is thus actually due to intra-guild predation (*de facto*, intra-guild cannibalism). Do we need a closure term? See Mitra (2008) for a discussion in the context of plankton ecology, though the arguments have wider ramifications.

11.9 Where Next

A major form of closure, given that most models describe functional groups rather than individual species, is intra-guild cannibalism. To implement this, and indeed other complex food web interactions, requires the use of appropriate prey selectivity functions. This is a highly complex arena, especially when linked (as it should be) to quality and quantity of prey options and to predator satiation. See Mitra & Flynn (2006a) and Flynn & Mitra (2016) for some discussion on these matters. See also Chapter 17.

12. A Classic Nutrient-Phytoplankton-Zooplankton Model

Terms and concepts introduced in this chapter- NPZ, series variable inputs, spin-up

12.1 Ecological Context

Two thirds of Earth is covered by the oceans. The bulk of the biological activity in the oceans, and indeed 50% of all planetary primary production, is mediated by the marine phytoplankton, controlled by a combination of nutrients, light and predation by the zooplankton, and other losses. Accepting that this is now recognised as a flawed simplification (as ca. 50% of the microplankton are mixotrophic – Flynn et al. 2013, Mitra et al. 2014, 2016) the oceans represent arguably the most important single, continuously linked, and well researched ecosystem on the planet.

In this chapter we will build and explore a classic description of oceanographic nutrient-phytoplankton-zooplankton (“NPZ”) interactions. The model described here was written by the late Prof Michael JR Fasham FRS, a father figure for the “NPZ” genera of marine models as applied to oceanography (the classic paper is Fasham et al. 1990). The naming of the variables is largely consistent with those used in the original description, though the structure has been modified slightly to conform to approaches developed in this book.

The ecology model is in essence similar to that we considered in Chapter 5 (Fig. 12.1)

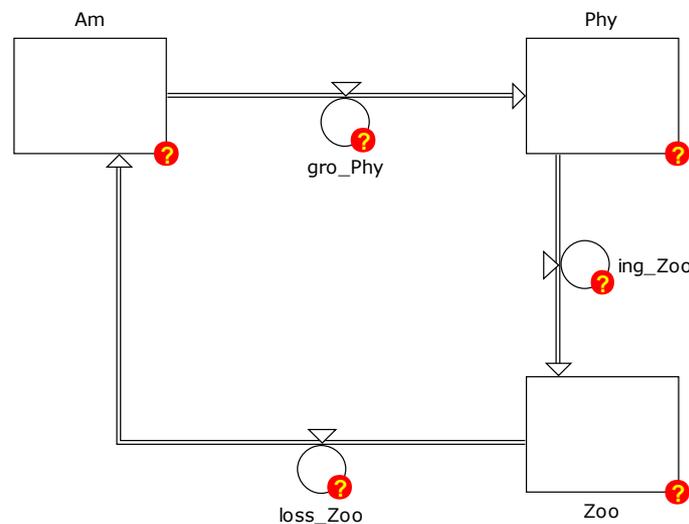


Fig. 12.1 Re-created from Fig. 5.1 as an initial conceptual nutrient-phytoplankton-zooplankton (“NPZ”) model.

However, we will now bring to this structure the following:

- dilutions in and out of the system (Chapter 7; akin here to mixing across the energy discontinuity, which here is a thermocline),
- density dependence with self-shading as the phytoplankton population grows (Chapter 8),
- seasonal changes in irradiance (Chapter 9),

- driving of physics through reference to external data sets (Chapter 10),
- death of the zooplankton (described through a closure term; Chapter 11).

In addition there are several other developments along the way.

The model runs for an oceanographic site in the North Atlantic, “NABE” (North Atlantic Bloom Experiment), which is at 47°N 20°W. The model comprises several sub-models, though in its entirety the model is simpler in its overall structure than that we considered when describing “pond life” in Chapter 10.

12.2 Mixing Module

The first part of the model describes the physical mixing between the upper mixed layer of the water column (which is lit by the sun and hence supports primary production) and the lower (unmixed, dark) layer. The depth of the mixed layer is here named *mix_dep*. These layers are separated by an ergocline, a zone of sharp energy difference typically associated with the thermocline.

Over the year the depth of *mix_dep* varies at the NABE station from a maximum of >300m deep in the winter, to a minimum in summer of around 15m. This change has profound effects on phytoplankton production as it holds the organisms closer to (or allows them to move further away from) the surface light. It is assumed that organisms in this mixed layer are homogeneously mixed.

The total mixing (*tot_mix*) comprises two components, one is that due to diffusive mixing (*dif_mix*) and the other is that due to changes in the mixed layer depth itself, as the physics alter with the seasons. The latter is of particular importance when depth is increasing as this event essentially entrains (brings into, or dilutes) the surface waters with nutrient-rich water from below the ergocline. To involve these processes together requires reference to input data for the mixing depth changing over the year.

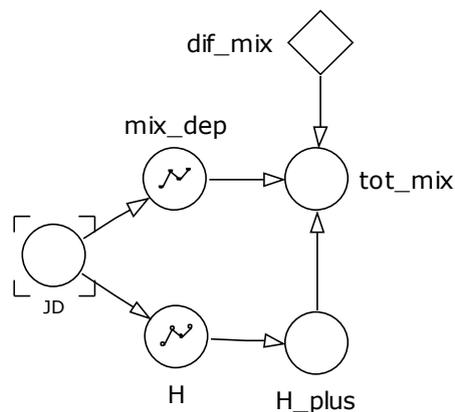


Fig. 12.2 Mixing module. See Table 12.1.

| Time | mix_dep | H |
|------|---------|-------|
| 0 | 218 | 4.6 |
| 5 | 239.6 | 4.32 |
| 10 | 261.1 | 4.3 |
| 15 | 282.7 | 4.32 |
| 20 | 287.5 | 0.96 |
| 25 | 287.5 | 0 |
| 30 | 288.2 | 0.14 |
| 35 | 288.9 | 0.14 |
| 40 | 289.5 | 0.12 |
| 45 | 290.2 | 0.14 |
| 50 | 290.9 | 0.14 |
| 55 | 294.4 | 0.7 |
| 60 | 298.9 | 0.9 |
| 65 | 303.1 | 0.84 |
| 70 | 307.3 | 0.84 |
| 75 | 311.7 | 0.88 |
| 80 | 316 | 0.86 |
| 85 | 306 | -2 |
| 90 | 296 | -2 |
| 95 | 286 | -2 |
| 100 | 276 | -2 |
| 105 | 266 | -2 |
| 110 | 256 | -2 |
| 115 | 160.5 | -19.1 |
| 120 | 65 | -19.1 |
| 125 | 26 | -7.8 |
| 130 | 20 | -1.2 |
| 135 | 20 | 0 |
| 140 | 20 | 0 |
| 145 | 20.1 | 0.02 |
| 150 | 20.3 | 0.04 |
| 155 | 20.5 | 0.04 |
| 160 | 20.6 | 0.02 |
| 165 | 20.8 | 0.04 |
| 170 | 21 | 0.04 |
| 175 | 20.2 | -0.16 |
| 180 | 19.3 | -0.18 |
| 185 | 18.3 | -0.2 |
| 190 | 17.3 | -0.2 |
| 195 | 16.4 | -0.18 |
| 200 | 15.4 | -0.2 |
| 205 | 15.7 | 0.06 |
| 210 | 16.8 | 0.22 |
| 215 | 17.9 | 0.22 |
| 220 | 19.1 | 0.24 |
| 225 | 20.2 | 0.22 |
| 230 | 21.3 | 0.22 |
| 235 | 22.4 | 0.22 |
| 240 | 23.4 | 0.2 |
| 245 | 24.4 | 0.2 |
| 250 | 25.4 | 0.2 |
| 255 | 26.4 | 0.2 |
| 260 | 27.4 | 0.2 |
| 265 | 28.8 | 0.28 |
| 270 | 30.7 | 0.38 |
| 275 | 32.6 | 0.38 |
| 280 | 34.6 | 0.4 |
| 285 | 36.5 | 0.38 |
| 290 | 38.5 | 0.4 |
| 295 | 41.2 | 0.54 |
| 300 | 47.4 | 1.24 |
| 305 | 53.6 | 1.24 |
| 310 | 59.7 | 1.22 |
| 315 | 65.9 | 1.24 |
| 320 | 72.1 | 1.24 |
| 325 | 79.3 | 1.44 |
| 330 | 90.9 | 2.32 |
| 335 | 102.5 | 2.32 |
| 340 | 114.2 | 2.34 |
| 345 | 125.8 | 2.32 |
| 350 | 137.4 | 2.32 |
| 355 | 149 | 2.32 |
| 360 | 172 | 4.6 |
| 365 | 195 | 4.6 |

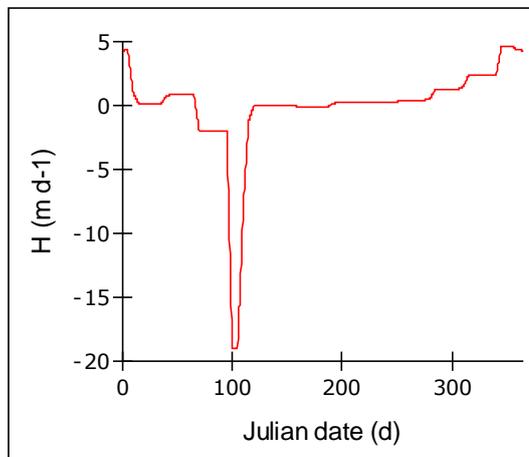
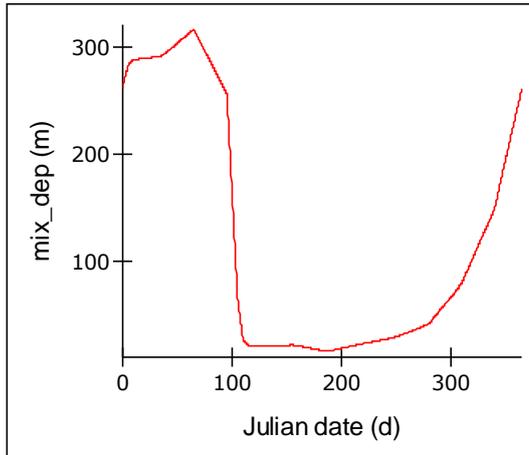


Fig. 12.3 Data describing *mix_dep* and *H*.

| Parameter | Type | Value | Unit | Description |
|----------------|------|--|-------------------|--|
| <i>dif_max</i> | Con | 0.18796 | m d ⁻¹ | Diffusive mixing |
| <i>JD</i> | Aux | {see Table 12.2} | d | Julian day, noting this repeats as TIME > 365, and the astronomic year starts on 21 st December |
| <i>H</i> | Aux | external data | m d ⁻¹ | Rate of change of mixed layer depth |
| <i>H_plus</i> | Aux | (H>0)*H | m d ⁻¹ | Selection of only +ve values of H |
| <i>mix_dep</i> | Aux | external data | m | Mixed layer depth against Julian date; note this is site-specific |
| <i>tot_mix</i> | Aux | (<i>dif_mix</i> + <i>H_plus</i>)/ <i>mix_dep</i> | d ⁻¹ | Total mixing across the ergocline |

Table 12.1 Equations for mixing module. See Fig. 12.2.

The data for mixing depth (*mix_dep*) come from oceanographic measurements at the NABE site (see Lochte et al. 1993). The rate of change in *mix_dep* is described by *H*. For example, over the first 5 days the mixing depth changes from 195 to 218 m (note that the data are assumed to wrap around, so the change for the first 5d of the year makes reference to the depth at the end of the previous year, assuming the cycle is strictly repeatable, which of course it would not be!). This gives a rate of change of (218-195)/5 m d⁻¹ = 4.6 m d⁻¹. These values are computed off line to generate the data series shown with Fig. 12.3.

The data are provided here in a tabulated form, together with plots (Fig. 12.3). From the latter you can see that the mixing depth decreases from a peak in winter of over 300m, to less than 20m over the summer. That is to say that plankton in the mixed layer could be randomly moved over a depth range that varies by an order of magnitude. You will need to use whatever approach is most appropriate for your chosen software platform to obtain reference to these data series.

Entries for these data series into Powersim Studio read as follows:

mix_dep=

```
GRAPH(JD,0,5,{218,239.6,261.1,282.7,287.5,288.2,288.9,289.5,290.2,290.9,294.4,298.8,303.1,307.4,311.7,316,306,296,286,276,266,256,160.5,65,26,20,20,20,20.1,20.3,20.5,20.6,20.8,21,20.2,19.3,18.3,17.3,16.4,15.4,15.7,16.8,17.9,19.1,20.2,21.3,22.4,23.4,24.4,25.4,26.4,27.4,28.8,30.7,32.6,34.6,36.5,38.5,41.2,47.4,53.6,59.7,65.9,72.1,79.3,90.9,102.5,114.2,125.8,137.4,149,172,195,218})
```

H=

```
GRAPH(JD,0,5,{4.60,4.32,4.30,4.32,0.96,0.14,0.14,0.12,0.14,0.14,0.70,0.88,0.86,0.86,0.86,-2.00,-2.00,-2.00,-2.00,-2.00,-19.10,-19.10,-7.80,-1.20,0.00,0.00,0.02,0.04,0.04,0.02,0.04,0.04,-0.16,-0.18,-0.20,-0.20,-0.18,-0.20,0.06,0.22,0.22,0.24,0.22,0.22,0.22,0.20,0.20,0.20,0.20,0.20,0.28,0.38,0.38,0.40,0.38,0.40,0.54,1.24,1.24,1.22,1.24,1.24,1.44,2.32,2.32,2.34,2.32,2.32,2.32,4.60,4.60,4.60})
```

Of equal importance to the value of *mix_dep* is the mixing rate. This is shown in Fig. 12.4.

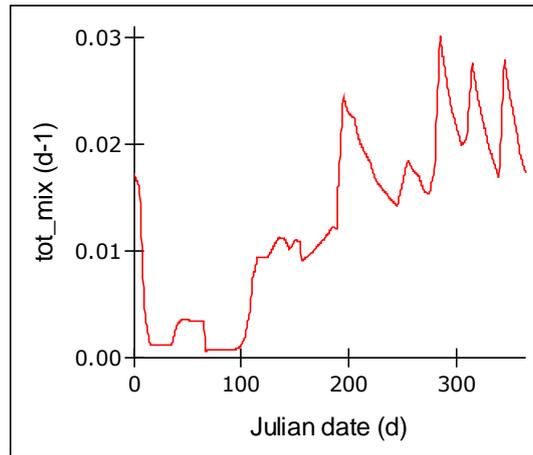


Fig. 12.4 Values of *tot_mix* from the mixing sub-model.

The value of *tot_mix* is akin to a dilution rate acting on the contents of the mixed layer (Cf. Chapter 7). Through reference to this value, nutrients from below the mixed layer are brought into the upper waters, while a proportion of biomass and residual nutrients are removed from it.

12.3 Irradiance and Photosynthesis Modules

The irradiance module is modified slightly from that in Chapter 9, with latitude set for 47° and a value for *atmos_clar* appropriate for this location (and which in this model is considered as a constant).

The output from the irradiance module, as *nat_PFD*, is coupled to a slightly modified light attenuation and depth-integrated photosynthesis module (Fig. 12.5; see Chapter 8). Care needs to be taken to adjust for different units because the main biological model operates in units of mmol N m^{-3} , and not in mass units. The water depth is now not fixed, but is described as changing with Julian date as described by the auxiliary *mix_dep*.

The output from the photosynthesis module is a co-nutrient-light-limited N-specific depth-integrated photosynthetic rate (and hence here, growth rate), *PSqz*. This value informs the main “NPZ” model structure. There is no phytoplankton respiration term in this variant of the “NPZ” model.

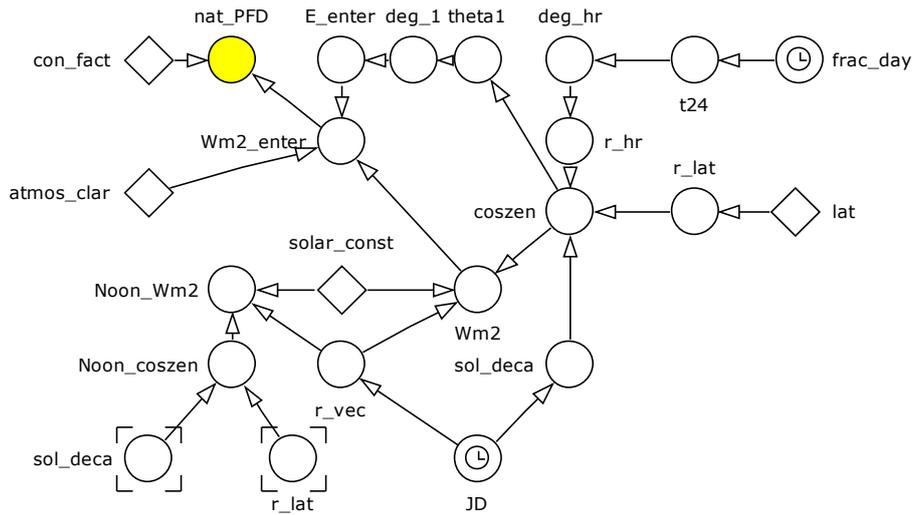


Fig. 12.5 Irradiance sub-model. See Table 12.2.

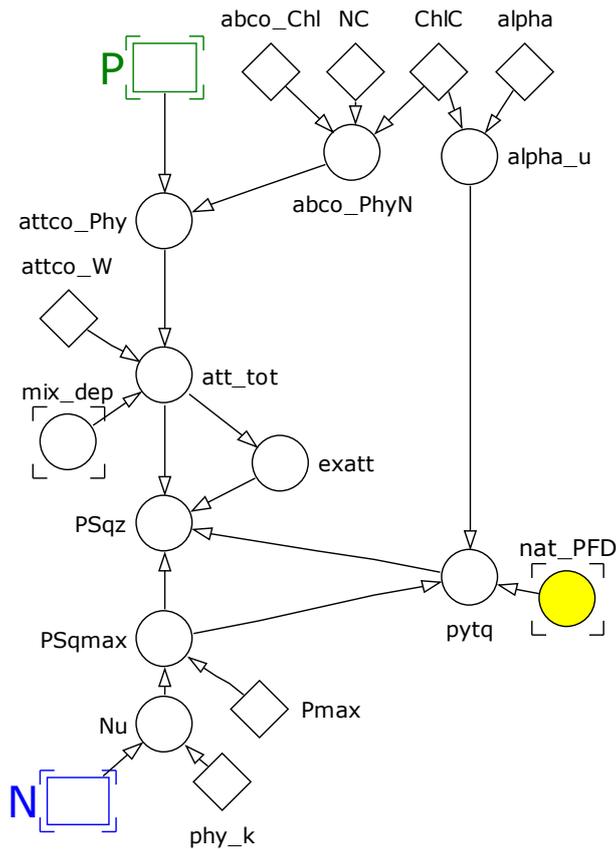


Fig. 12.6 Phytoplankton growth module. See Table 12.3.

| Variable | Type | Value | Unit | Description |
|--------------------|------|---|---|--|
| <i>atmos_clar</i> | Con | 0.38 | dl | Corrects for atmospheric clarity (varies with lat, long & JD) |
| <i>con_fact</i> | Con | 4.57 | dl | Converts W m ⁻² to PAR μmol m ⁻² s ⁻¹ for cloud-less sky with sun |
| <i>lat</i> | Con | 47 | ° | Latitude |
| <i>solar_const</i> | Con | 1368 | Wm ⁻² | Solar constant irradiance (Wm ⁻² = J/m ² /s); maximum irradiance to Earth from the sun |
| <i>coszen</i> | Aux | $\text{MAX}(\text{SIN}(r_lat)*\text{SIN}(sol_deca)+\text{COS}(r_lat)*\text{COS}(sol_deca)*\text{COS}(r_hr),0)$ | dl | Cosine of zenith angle; positive values only accepted |
| <i>deg_1</i> | Aux | $(theta1 * 1.0 \ll \text{deg/rad} \gg)$ | ° | Angle the sun makes with the vertical (solar zenith angle) |
| <i>deg_hr</i> | Aux | $\text{ABS}(12-t24)*15$ | dl | Degrees of hour angle away from noon (default 12:00) |
| <i>E_enter</i> | Aux | $1-(1.15\text{E-}06*deg_1^3 - 6.9134\text{E-}05*deg_1^2 + 0.001*deg_1 + 0.0187)$ | dl | Proportion of light incident with the water surface that is just under the surface, accounting for reflectance |
| <i>frac_day</i> | Aux | $\text{FRAC}(\text{TIME})$ | dl | Current time as fraction of day |
| <i>JD</i> | Aux | $(sw_JD=1)*(365*(\text{FRAC}((\text{TIME}+10)/365)))+(sw_JD=0)*set_JD$ | d | Julian day; note the 10d offset (starting the year on 22 nd December) |
| <i>nat_PFD</i> | Aux | $Wm2_enter*con_fact$ | μmol photon m ⁻² s ⁻¹ | PFD just under surface |
| <i>noon_coszen</i> | Aux | $\text{MAX}(\text{SIN}(r_lat)*\text{SIN}(sol_deca)+\text{COS}(r_lat)*\text{COS}(sol_deca)*\text{COS}(0),0)$ | dl | Value of coszen at noon (hence COS(0) at end of definition) |
| <i>noon_Wm2</i> | Aux | $solar_const/r_vec/r_vec*Noon_coszen$ | W m ⁻² | Maximum irradiance (at noon) on this Julian date |
| <i>r_hr</i> | Aux | $deg_hr*\text{PI}/180$ | rad | Hour angle radians |
| <i>r_lat</i> | Aux | $lat*\text{PI}/180$ | rad | Latitude in radians |
| <i>r_vec</i> | Aux | $1/(1+0.033*\text{COS}(2*\text{PI}*JD*0.00274))^0.5$ | | Earth radius vector |
| <i>sol_deca</i> | Aux | $23.45*\text{SIN}(2*\text{PI}*(284+JD)*0.00274)*\text{PI}/180$ | rad | Solar declination angle |
| <i>t24</i> | Aux | $24*frac_day$ | hrs | Current time as fraction of day in hours |
| <i>theta1</i> | Aux | $\text{ARCCOS}(coszen)$ | rad | Angle the sun makes with the vertical (solar zenith angle) |
| <i>Wm2</i> | Aux | $solar_const/r_vec/r_vec*coszen*(coszen>0)$ | W m ⁻² | Irradiance at given hour and day; W m ⁻² [W = J s ⁻¹ ; i.e. J/m ² /s] |
| <i>Wm2_enter</i> | Aux | $Wm2*E_enter*atmos_clar$ | W m ⁻² | Light actually entering water (just under surface), accounting for reflectance |

Table 12.2 Description of astronomical light, including the effect of reflectance at the water surface.

| Variable | Type | Value | Unit | Description |
|--------------|------|--|---|--|
| N | SV | {see Table 12.4} | mmol N m ⁻³ | Nutrient-N |
| P | SV | {see Table 12.4} | mmol N m ⁻³ | Phytoplankton biomass-N |
| $abco_Chl$ | Con | 0.02 | m ² (mg Chl) ⁻¹ | Light absorbance coefficient for chlorophyll |
| $alpha$ | Con | 7e-6 | (m ² g ⁻¹ Chl)*(gC μmol ⁻¹ photon) | Slope of Chl-specific PE curve |
| $attco_W$ | Con | 0.0323 | m ⁻¹ | Absorbance coefficient for growth medium (water) |
| $ChlC$ | Con | 0.06 | gChl gC ⁻¹ | Mass ratio content of chlorophyll:C in the phytoplankton |
| NC | Con | 0.15 | gN gC ⁻¹ | Mass ratio content of N-biomass:C in the phytoplankton |
| phy_k | Con | 0.5 | mmol N m ⁻³ | Half saturation constant for Nu |
| $Pmax$ | Con | 0.5 | gN gN ⁻¹ d ⁻¹ | Phytoplankton maximum N-specific growth rate (actually the maximum photosynthetic rate in N-units) |
| $abco_PhyN$ | Aux | $abco_Chl * ChlC/NC$ | m ² (mgN) ⁻¹ | Phytoplankton-N specific coefficient for light absorbance |
| $alpha_u$ | Aux | $alpha * ChlC$ | (m ²)*(μmol ⁻¹ photon) | Specific slope of PE curve |
| $attco_Phy$ | Aux | $abco_PhyN * P * 14$ | m ⁻¹ | Attenuation coefficient to phytoplankton N-biomass; note correction of units from moles to mass by *14 |
| att_tot | Aux | $mix_dep * (attco_W + attco_Phy)$ | dl | Total attenuation |
| $exatt$ | Aux | $EXP(-att_tot)$ | dl | Negative exponent of total attenuation |
| mix_dep | Aux | {see Table 12.1} | m | Mixed layer depth |
| nat_PFD | Aux | {see Table 12.2} | μmol photon m ⁻² s ⁻¹ | Surface irradiance (see text) |
| Nu | Aux | $N/(N+phy_k)$ | dl | Index of N-limitation |
| $PSqmax$ | Aux | $pmax * Nu$ | d ⁻¹ | Maximum photosynthetic rate down-regulated in consequence of nutrient stress |
| $PSqz$ | Aux | $pqmax * (LN(py tq + SQRT(1 + py tq^2)) - LN(py tq * exatt + SQRT(1 + (py tq * exatt)^2))) / att_tot$ | d ⁻¹ | Phytoplankton depth integrate N-specific growth rate |
| $py tq$ | Aux | $(alpha_u * PFD * 24 * 60 * 60) / pqmax$ | d | Intermediate in depth-integrated photosynthesis rate |

Table 12.3 Equations for coupled nutrient-light limited phytoplankton growth module.

12.4 The Main “NPZ” Module

The main NPZ model structure is shown in Fig. 12.7, with equations in Table 12.4. It is important to note that the base unit for this model is moles, not mass. Thus, the state variables have units of mmol N m⁻³; this is the same as μmol N L⁻¹, and hence for dissolved nutrients equates to μM.

We will now go through this structure, commencing with nutrients.

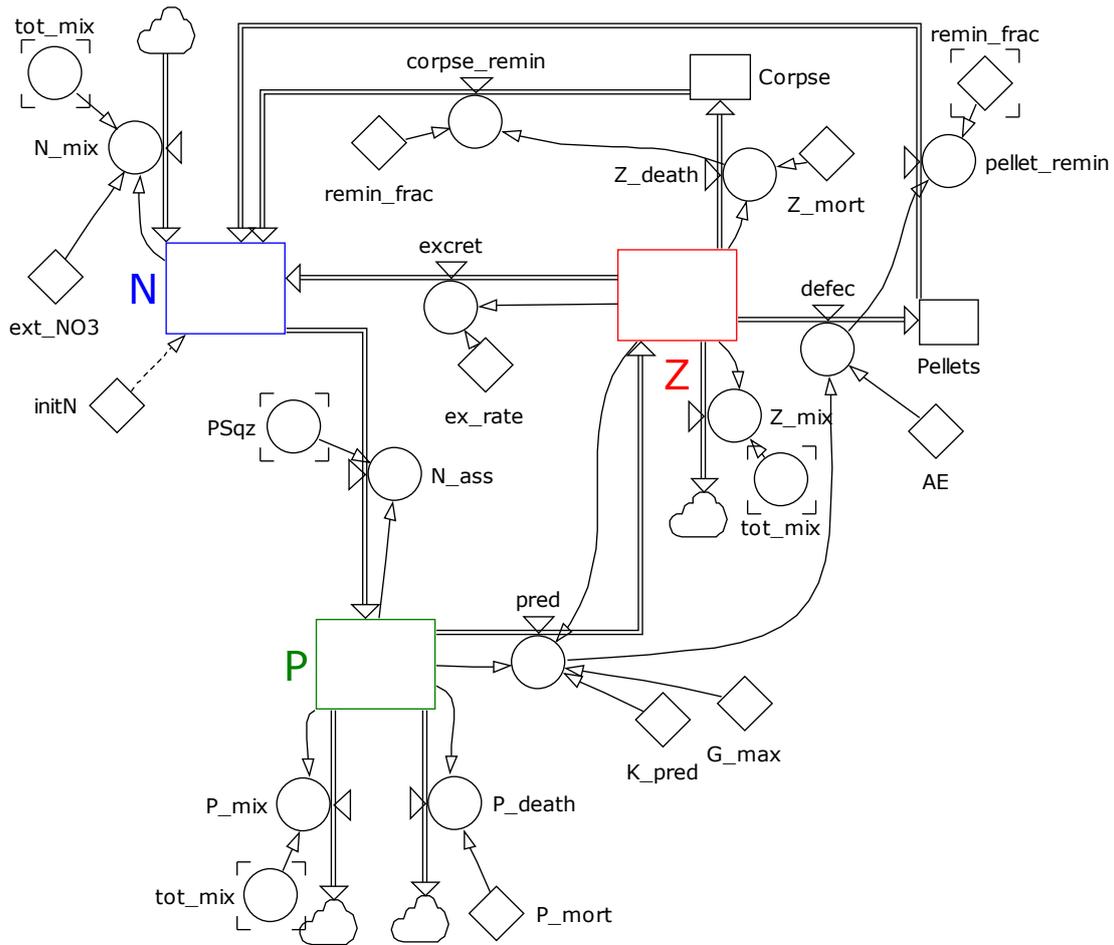


Fig. 12.7 Main Nutrient-Phytoplankton-Zooplankton model. See Table 12.4.

The nutrient state variable (N) functionally include both nitrate (which enters according to the rate set by tot_mix from below the mixed layer, where is present at a concentration defined by ext_NO3) and also ammonium regenerated by the biota within the mixed layer ecosystem.

Nutrient (N), together with light (nat_PFD accounting for attenuation) limits the growth of phytoplankton (P) as defined by $PSqz$ (see Fig. 12.6). This defines the phytoplankton population growth in terms of assimilated N , as N_ass . The phytoplankton are subjected to mixing out (akin to a chemostat washout) from the mixed layer (P_mix). They are also subjected to death (P_death), and also by grazing by the zooplankton ($pred$). In reality P_death could be attributed to various factors, such as sedimentation and viral lysis.

| Variable | Type | Value | Unit | Description |
|---------------------|------|---|---------------------------------------|--|
| <i>Corpse</i> | SV | 0 + <i>Z_death</i> - <i>corpse_remin</i> | mmol Nm ⁻³ | Corpse N-biomass lost from system; records cumulative loss |
| <i>N</i> | SV | <i>initN</i> + <i>excret</i> + <i>pellet_remin</i> + <i>corpse_remin</i> + <i>N_mix</i> - <i>N_ass</i> | mmol Nm ⁻³ | Dissolved Inorganic-N (nitrate + ammonium) |
| <i>P</i> | SV | 0.09 + <i>N_ass</i> - <i>pred</i> - <i>P_mix</i> - <i>P_death</i> | mmol Nm ⁻³ | Phytoplankton N-biomass |
| <i>pellets</i> | SV | 0 + <i>defec</i> - <i>pellet_remin</i> | mmol Nm ⁻³ | Zooplankton faecal pellets; records cumulative loss |
| <i>Z</i> | SV | 0.029 + <i>pred</i> - <i>excret</i> - <i>defec</i> - <i>Z_death</i> | mmol Nm ⁻³ | Zooplankton N-biomass |
| <i>AE</i> | Con | 0.75 | dl | Assimilation efficiency |
| <i>ex_rate</i> | Con | 0.05 | d ⁻¹ | Excretion rate (=regeneration) |
| <i>ext_NO3</i> | Con | 7.25 | mmol Nm ⁻³ | Nitrate concentration below mixed layer |
| <i>G_max</i> | Con | 0.59 | d ⁻¹ | Maximum N-specific grazing rate of zooplankton on phytoplankton |
| <i>initN</i> | Con | 5.6 | mmol Nm ⁻³ | Initial value for N |
| <i>K_pred</i> | Con | 0.76 | mmol Nm ⁻³ | Half saturation constant for predation |
| <i>P_mort</i> | Con | 0.05 | d ⁻¹ | Mortality rate for phytoplankton |
| <i>remin_frac</i> | Con | 0.167 | dl | Fraction remineralised |
| <i>Z_mort</i> | Con | 0.56 | dl | Closure constant |
| <i>corpse_remin</i> | Aux | <i>Z_death</i> * <i>remin_frac</i> | mmol Nm ⁻³ d ⁻¹ | Remineralisation of zooplankton corpses to nutrient-N within mixed layer |
| <i>defec</i> | Aux | (1- <i>AE</i>)* <i>pred</i> | mmol Nm ⁻³ d ⁻¹ | Defecation by zooplankton |
| <i>excret</i> | Aux | <i>Z</i> * <i>ex_rate</i> | mmol Nm ⁻³ d ⁻¹ | Regeneration of N by zooplankton |
| <i>N_ass</i> | Aux | <i>P</i> * <i>PSqz</i> | mmol Nm ⁻³ d ⁻¹ | N-assimilation by phytoplankton |
| <i>N_mix</i> | Aux | <i>ext_NO3</i> * <i>tot_mix</i> | mmol Nm ⁻³ d ⁻¹ | Nitrate input and nutrient-N output |
| <i>P_death</i> | Aux | <i>P</i> * <i>P_mort</i> | mmol Nm ⁻³ d ⁻¹ | Loss of phytoplankton by death |
| <i>P_mix</i> | Aux | <i>P</i> * <i>tot_mix</i> | mmol Nm ⁻³ d ⁻¹ | Removal of phytoplankton by mixing |
| <i>pellet_remin</i> | Aux | <i>defec</i> * <i>remin_frac</i> | mmol Nm ⁻³ d ⁻¹ | Remineralisation of faecal pellets |
| <i>pred</i> | Aux | <i>Z</i> * <i>G_max</i> * <i>P</i> /(<i>P</i> + <i>K_pred</i>) | mmol Nm ⁻³ d ⁻¹ | Grazing rate by zooplankton on phytoplankton |
| <i>PSqz</i> | Aux | {see Table 12.3} | d ⁻¹ | N-specific phytoplankton growth rate |
| <i>tot_mix</i> | Aux | {see Table 12.1} | d ⁻¹ | Total mixing across the ergocline |
| <i>Z_death</i> | Aux | <i>Z_mort</i> *(<i>Z</i> ²) | mmol Nm ⁻³ d ⁻¹ | Closure term on zooplankton |
| <i>Z_mix</i> | Aux | <i>Z</i> * <i>tot_mix</i> | mmol Nm ⁻³ d ⁻¹ | Removal of zooplankton by mixing |

Table 12.4 Equations for main Nutrient-Phytoplankton-Zooplankton model. See Fig. 12.7.

The grazing function within *pred* describes a rectangular hyperbolic relationship between phytoplankton abundance (*P*), with half saturation constant (*K_pred*), and a N-specific maximum grazing rate (*G_max*). The population grazing rate (*pred*) links this N-specific prey-abundance rate to the zooplankton abundance (*Z*). Note that here, the maximum growth rate of the zooplankton is an emergent property of ingestion minus loss; there is no stated maximum growth rate for the zooplankton as we used in Chapter 5.

The phytoplankton biomass that enters the zooplankton may be incorporated into new biomass, voided through defecation (*defec*) to *Pellets* assuming a fixed assimilation efficiency (*AE*), or excreted during regeneration (*excret*) associated with respiration (*ex_rate*). The zooplankton biomass itself may be mixed out of the mixed layer (*Z_mix*) and thus in reality (not modelled) support the growth of organisms living in deep waters. Zooplankton are also subjected to predation from higher trophic levels; this is described through a closure function (see Chapter 11), which in this instance is a quadratic term (*Z_death*, with constant *Z_mort*).

Of the faecal *Pellets*, a proportion (*remin_frac*) are assumed to be rapidly remineralised back to nutrient-N (*N*) within the mixed layer (*pellet_remin*); the remainder is lost by sedimentation with state variable *Pellets* recording the cumulative loss. A similar fate befalls *Corpse*, with the same *remin_frac* assumed to be converted to nutrient-N within the mixed layer, with *Corpse* recording the cumulative loss.

While the N-specific growth rate of the phytoplankton (*PSqz*) is already computed, the growth rate of the zooplankton is not used in the model. Nonetheless, it is of interest to compute it. The growth rate, *Zu*, and also the grazing rate, are given using Fig. 12.8 and Table 12.5.

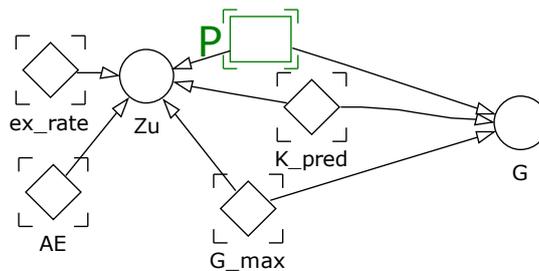


Fig. 12.8 N-specific zooplankton growth and grazing rates. See Table 12.5.

| Variable | Type | Value | Unit | Description |
|----------------|------|---|------------------------|---|
| <i>P</i> | SV | {see Table 12.4} | mmol N m ⁻³ | Phytoplankton biomass-N |
| <i>AE</i> | Con | {see Table 12.4} | dl | Assimilation efficiency |
| <i>ex_rate</i> | Con | {see Table 12.4} | d ⁻¹ | Excretion rate (=regeneration) |
| <i>G_max</i> | Con | {see Table 12.4} | d ⁻¹ | Maximum N-specific grazing rate of zooplankton on phytoplankton |
| <i>K_pred</i> | Con | {see Table 12.4} | mmol Nm ⁻³ | Half saturation constant for predation |
| <i>G</i> | Aux | $G_{max} * P / (P + K_{pred})$ | d ⁻¹ | N-specific grazing rate |
| <i>Zu</i> | Aux | $(G_{max} * (P / (P + K_{pred})) * AE) - ex_{rate}$ | d ⁻¹ | N-specific zooplankton growth rate |

Table 12.5 Equations for N-specific zooplankton growth and grazing rates. See Fig. 12.8.

12.5 Parameterising the Model

Source field data and additional information for this particular simulation are given in Lochte et al. (1993) and Fasham et al. (1990). The value for the constants are derived through the use of a tuning methodology which will be described in detail in Chapter 14.

12.6 Operating the Model

Some example output is given in Figs. 12.9 – 12.12. The real ecosystem dynamics, even as represented here using a simple model, can be seen to be highly complex, linking seasonal drivers of mixing depth and light availability together with predator-prey interactions and nutrient recycling.

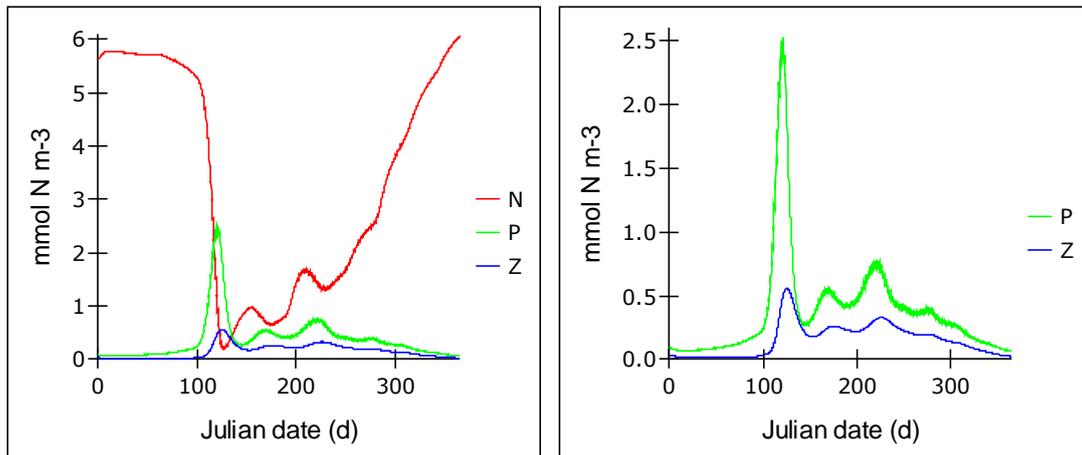


Fig. 12.9 Changes in allocation of nutrient-N between nitrate+ammonium (N), phytoplankton (P) and zooplankton (Z) over the Julian year.

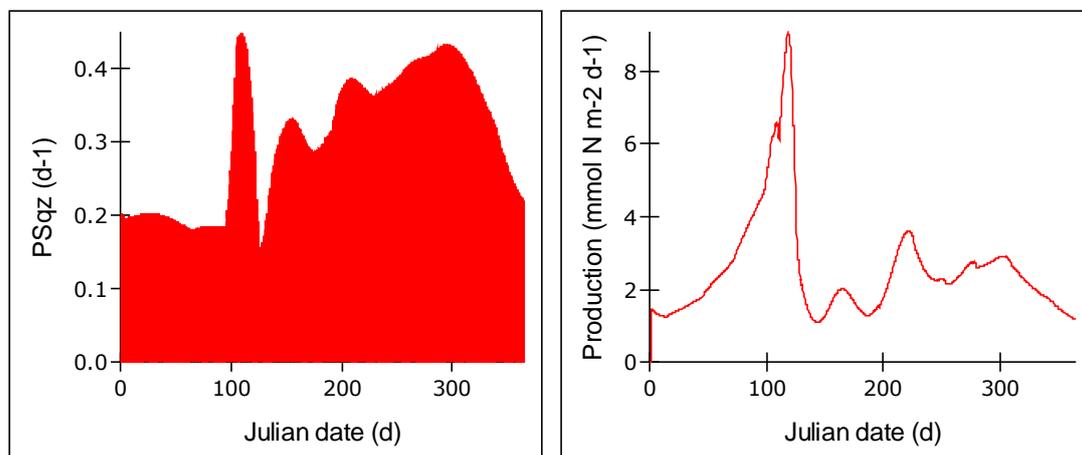


Fig. 12.10 Changes in phytoplankton growth rate ($PSqz$) and in areal production over the Julian year. The plot for $PSqz$ appears as it does in consequence of the light-dark cycle, there being no photosynthesis at night. The production plot is obtained by taking the value of N_{ass} (which is a production rate per m^3 per day) and multiplying by the mixed layer depth (mix_dep).

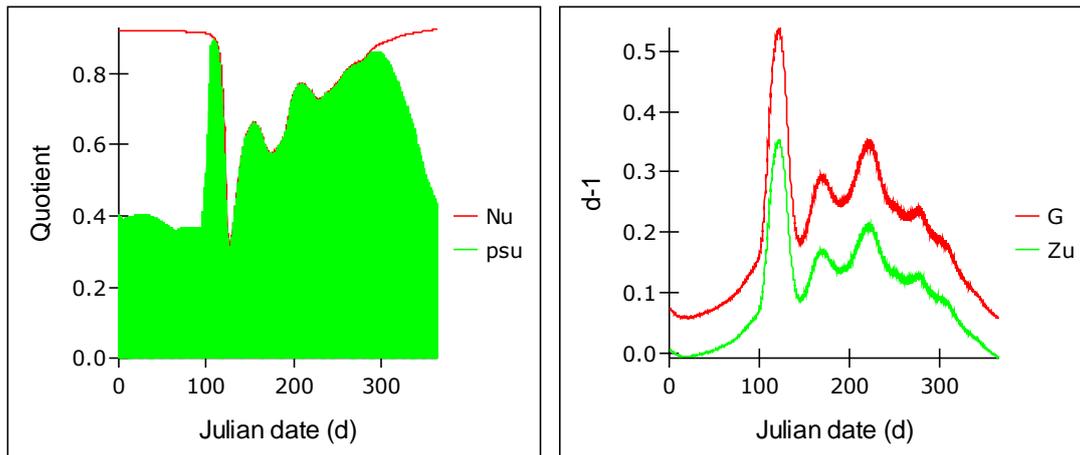


Fig. 12.11 Changes in factors affecting growth rates for phytoplankton and zooplankton over the Julian year. The value of psu describes the state of coupled nutrient-light limitation of phytoplankton growth (a value of 1 being optimal). Until ca. day 100 nutrient availability alone (indicated by Nu) is not limiting; it remains co-limiting with light until the end of ca. day 280. The grazing rate (G) is so low during the winter that the net growth rate of zooplankton (Zu) is negative. Zooplankton growth rate (Zu) is high over the summer when the phytoplankton are typically nutrient rather than light limited; although nutrient-limited phytoplankton would be of lower nutritional value as feed, there is no linkage in this model of feeding to food quality with which to explore the interaction (see Mitra et al. 2007 and also Chapter 17).

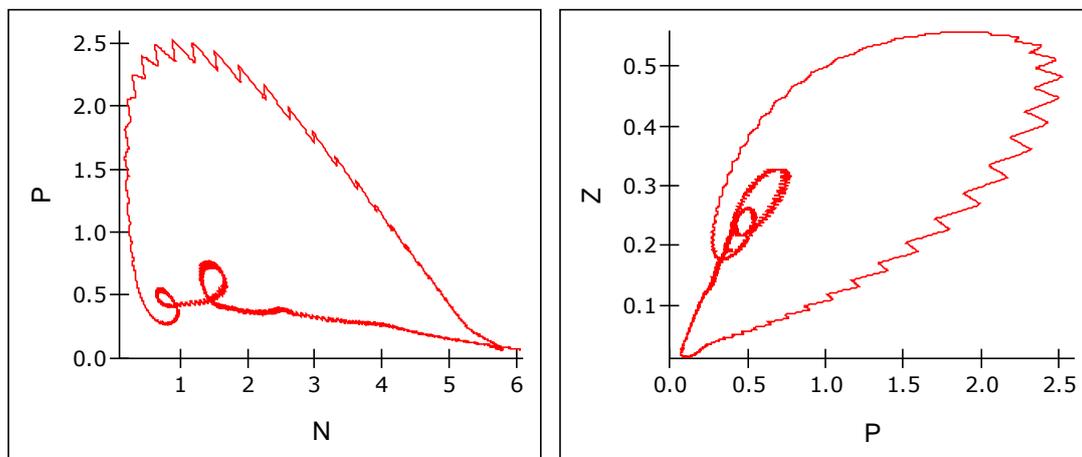


Fig. 12.12 Plots of nutrient (N) vs phytoplankton (P), and phytoplankton (P) versus zooplankton (Z), showing the nonlinearities in the relationships. These are driven by oscillations in predator-prey interactions, coupled with the influence of nutrient cycling, all affected by a strong set of seasonal drivers.

12.6 Things to Explore

For all of the following, run the model over several years (e.g. 3×365 days); the runs will converge with time to give a repeatable annual cycle, so you should really look at the last year's simulation. This process is called **spin-up**, and is needed when running ecosystem models that take some time to reach a quasi-steady-state condition, where behaviour within a given set of external drivers (here, light and mixing depth) gives a repeatable pattern.

- i) Try running the model with different values of the constants controlling phytoplankton and zooplankton growth.
- ii) Try altering the sub-mixed layer nitrate concentration (*ext_NO3*) and/or the description of the mixed layer depth (*mix_dep*), and/or the latitude (*lat*) and *atmos_clar* values – how sensitive is the behaviour to such changes?
- iii) Think how changes brought about by climate change, or changes in water currents that shift the geographic centre of primary production and fisheries, may affect planktonic production.
- iv) Introduce some new auxiliaries to calculate the gC-specific areal production rate (i.e. convert the production in terms of $\text{mmol N m}^{-2} \text{d}^{-1}$ to $\text{gC m}^{-2} \text{d}^{-1}$, noting that the phytoplankton mass N:C is assumed here to be 0.15).
- v) If fisheries that consumed zooplankton were harvested (which here would alter the closure term, *Z_mort*, by decreasing it), what happens to total primary productivity?
- vi) Compute and plot the seasonal rates of production of material that sediments out of the mixed layer (i.e. the accumulation of *Pellets* and *Corpse*). Be careful to consider the role of the mixed layer depth in such calculations.
- vii) Go through the whole model critically reviewing each process, identifying aspects that could be improved, or otherwise enhanced. Mitra et al. (2007) consider some of the problems inherent in this particular model structure.

12.7 Caveats

As complexity in model structure increases, so the list of caveats increases. Some are more profound than others though, and may include the following:

- This is a ½D representation of what would perhaps ideally be considered as a 3D simulation (see Section 2.10). There are thus exchanges laterally throughout the water column that are not recognised here.
- The weather varies greatly year by year, so we may question the relative timing and magnitude of changes in the mixing depth that so greatly affects the overall dynamic.
- The biological model is very simple on very many fronts: ammonium and nitrate are lumped together as one N-source; silicate (an essential nutrient for diatoms) is not described; the seasonal progression through fundamentally different plankton types is not considered; variable stoichiometry and acclimative photobiology is ignored; mixotrophy is ignored.

That the model does as well as it does in comparison to the source data (see Chapter 14) partly reflects that various “wrongs” counter balance each other (see Mitra et al. 2007). That is also a warning that increasing detail in sub-models needs to be undertaken with care and in a balanced way.

12.8 Where Next

In Chapters 13 and 14 we consider how sensitive is this model structure to the choice of input variables, and also how those input variables may be tuned to achieve the best fit of the model to data.

13. Sensitivity (Risk) Analyses

Terms and concepts introduced in this chapter- sensitivity vs risk analysis, steady-state vs dynamic analysis

13.1 Ecological Context

Biology and thence ecology represent immensely complex adaptive systems. While molecular biology has shown that biology contains even more variability than we suspected, models lump not only individuals of one species together, but most often they lump very diverse groups together into what are termed functional types (e.g., Weithoff 2003). So the functional type we term “phytoplankton” includes any and all phototrophic microscopic organisms, including such diverse groups as cyanobacteria, diatoms, nanoflagellates, dinoflagellates, foraminifera etc. Such groups inevitably encompass allometric (size) ranges covering several orders of magnitude, together with growth rates and nutrient affinities etc. also covering a wide range. Yet in models we typically use single fixed values for the maximum growth rate, for the nutrient affinity, for prey affinity as viewed by a single predator functional group, a predator grouping which itself similarly covers a massive range in size and activities. How can we judge whether our simulations have any useful meaning at all, and what may be the boundaries to our understanding?

Two factors affect the ability of a model output to match reality; one is the model structure (how the flows between the defined state variables are described by equations), and the other is the value of input variables (“constants”) used to drive the equations in the structure. This assumes, of course, that suitable data are available in the first instance upon which to make comparisons (i.e., data that are reliable and representative of the system, that are available in appropriate units, and with sufficient temporal resolution). However, an important confounding issue is that of sensitivity of the model to the choice of parameter values for constants. In this chapter we consider the subject of model sensitivity; we consider the issue of matching model behaviour to reality in Chapter 14.

Some refer to sensitivity analysis as an analysis of risk; that is an assessment of the likelihood of the model giving a certain output if we do not get the input values spot on. Risk analysis is of particular interest in economic models; if you get the cost estimate for the raw materials bill wrong by 5%, does the company go bankrupt? The basic question then, is how important is it to correctly set the values of constants that affect model behaviour?

For some variables that are held as constants we may have high confidence (e.g., temperature in a constant-temperature chamber, transforms of protein concentration to gN), while for others we have very little confidence that the (so-called constant) value is ever constant; this applies for example to maximum growth rate and assimilation efficiency values. If we use a value of such a constant that is incorrect by 50%, how does this affect the output? Is the output affected by a similar magnitude? For example, in the example of 50%, is the output also halved (i.e., $\times 0.5$) or doubled (i.e. $\times 1/0.5$)?

This is important in two other respects. Over-sensitivity (e.g., our 50% change results in a 10 fold change in output) may indicate a structural problem in the formulation of the model. Alternatively it could, of course, be indicative of a heightened sensitivity in this component in the real world. Either way, it is as well to check. In contrast, a very low sensitivity (e.g. our 50% change results in a

change in output by 0.01 fold) may indicate that the component making reference to the constant is of so little consequence that we may safely delete it. If we have high confidence in the model structure we can thus use a sensitivity analysis to help us simplify the model structure. This would be analogous to the complex-to-simple approach used in engineering; for example over-engineering the structure of a bridge, and then removing specific structural members that are actually of little or no consequence, confident that the remaining components will retain a robust functional structure.

We will consider two forms of sensitivity analysis – single parameter analysis conducted under steady-state conditions, and a dynamic analysis that may be conducted on one or many parameters simultaneously. In both instances for a working example we shall explore components of the “NPZ” model used in Chapter 12.

13.2 Single Parameter Sensitivity Analysis

Single parameter sensitivity analyses is performed using Eq.13.1 (Haefner 1996).

$$S = \frac{(Ra-Rn)/Rn}{(Pa-Pn)/Pn} \quad \text{Eq.13.1}$$

Here, Rn and Ra are the model outputs (responses) for the usual (nominal; Rn) and altered (Ra) model runs, when employing the nominal (Pn) or altered (Pa) constant input values.

The analysis reports a sensitivity index, S . A value of $S=0$ indicates no change in model output (Ra) with changes in input value (Pa). A result of $S=1$ indicates a pro rata change; that is a doubling in the input value doubles the output value. A result of $S= -0.5$ indicates a halving of output for a doubling of the input value.

Typically the analysis is conducted by considering a halving and doubling of each constant value from its nominal (Pn) value. Values of S beyond the range of -0.5 to 1 indicate heightened sensitivity. Whether that is of concern depends on the role of the variable in question, and how easily it is to accurately estimate its value in the real world. For biological systems, rate estimates and values relating to rate processes (such as half saturation constants) are particularly problematic in this regard.

The analysis should be conducted on a model running at steady-state. How do we do that on the structure that we are considering (the “NPZ” model in Chapter 12), driven as it is by a set of external factors (seasonal sunlight and mixed layer depths)? The answer is that the analysis cannot be conducted on the whole model. Further, because of the cyclic nature of the nutrient-phytoplankton-zooplankton interaction, an analysis of the sensitivity of, for example, a single parameter in the phytoplankton model, is also confounded by many other factors.

It is easiest to extract the subcomponent (e.g., phytoplankton, or zooplankton) and explore its behaviour alone. *Is that not cheating?*, you may ask. Well, an analogy would be testing each component of a car before putting it all together, and then testing the whole vehicle. For modelling, a steady-state single parameter sensitivity analysis is conducted on each part, and then the dynamic multi-parameter analysis is conducted on the whole system (Section 13.4). Taking the analogy forward, we can well imagine that the steady-state analysis would be best conducted with

the component operating under stress; you cannot judge the adequacy of a particular type of metal alloy for a bolt without placing the bolt under some form of loading.

Let us first consider the phytoplankton model. Growth of the phytoplankton in the NPZ model (Chapter 12) is controlled by light and nutrient availability. The constants that affect phytoplankton growth are given in Table 13.1, together with some plausible values.

| Variable | Type | Value | Unit | Description |
|--------------|------|-------|---|--|
| <i>Alpha</i> | Con | 3e-6 | (m ² g ⁻¹ Chl)*(gC μmol ⁻¹ photon) | Slope of Chl-specific PE curve |
| <i>ChlC</i> | Con | 0.03 | gChl (g C) ⁻¹ | Mass ratio content of chlorophyll:C in the phytoplankton |
| <i>NC</i> | Con | 0.15 | gN (g C) ⁻¹ | Mass ratio content of N-biomass:C in the phytoplankton |
| <i>Pmax</i> | Con | 0.5 | gN (gN) ⁻¹ d ⁻¹ | Phytoplankton maximum N-specific growth rate (actually the maximum photosynthetic rate in N-units) |
| <i>phy_k</i> | Con | 0.5 | mmol N m ⁻³ | Half saturation constant for <i>phy_u</i> |

Table 13.1 Constants directly involved in phytoplankton growth.

For the test we can propose the values given in Table 13.2. It is important, when selecting mid, low and high values, to consider plausible values only. Thus, for example, cellular N:C (NC, by mass) should be between ca. 0.05 – 0.2.

| Variable | Nominal value (Pn) | Low altered value (Pa ₁) | High altered value (Pa ₂) |
|--------------|--------------------|--------------------------------------|---------------------------------------|
| <i>Alpha</i> | 3e-6 | 1.5e-6 | 7e-6 |
| <i>ChlC</i> | 0.03 | 0.015 | 0.07 |
| <i>NC</i> | 0.1 | 0.05 | 0.2 |
| <i>Pmax</i> | 0.5 | 0.25 | 1 |
| <i>phy_k</i> | 0.5 | 0.25 | 1 |

Table 13.2 Test values.

To these we need to consider the input values of light and nutrient; we need to select values of these that stress the output. The value for nutrient (*N*) can be reliably set at broadly equal to the original *phy_k*, as by definition that quantity will only allow half the maximum growth rate. And we can set the biomass of P at some appropriate value selected from the model run. Let us consider the following:

- Fixed nutrient level (*N_fix*) at 0.5 or 2 mmol N m⁻³
- Fixed phytoplankton level (*P_fix*) at 2 or 0.5 mmol N m⁻³.
- Fixed mixed layer depth (*mix_dep_fix*) at 50m,
- Fixed light (*PFD_fix*) as a continuous set value of 1000 μmol photon m⁻² s⁻¹.

So, all that remains is to take just the phytoplankton component from the NPZ model, configure it with a fixed supply of N (i.e., one of the options listed as N_{fix} , above) and PFD (i.e., $PFD_{fix} = 1000$, as above), and compute the growth rate, $PSqz$. In this instance, we could do this on a spreadsheet, as we just need to steady-state $PSqz$ value, and if we remove all linkage to seasonality, mixing depth and the other components of the “NPZ” system (including not allowing P to increase), then the value of $PSqz$ will be constant. However, it is easy enough (and saves rebuilding the equations elsewhere) to just use the model structure. The stripped version of the phytoplankton growth component of the NPZ model now looks like this:

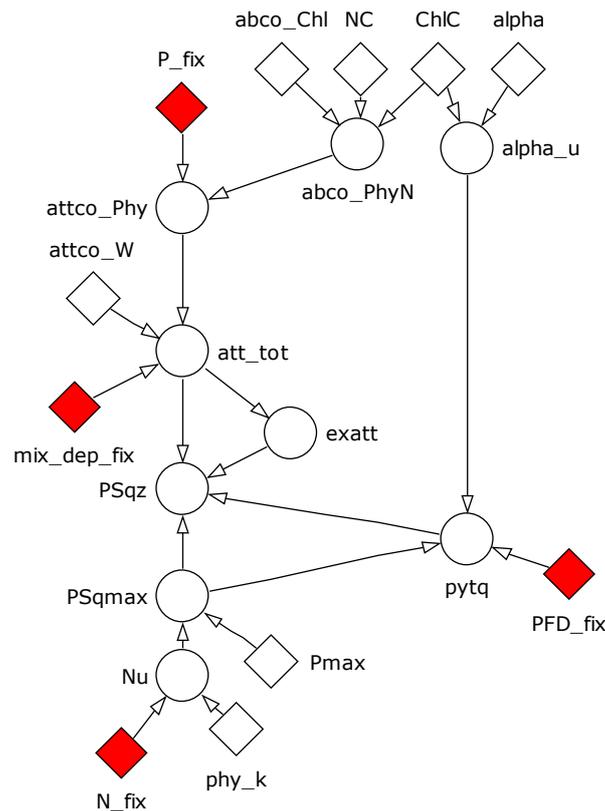


Fig. 13.1 Description of phytoplankton specific growth rate ($PSqz$) configured for steady-state sensitivity analysis. Symbols in red, which were input variables controlled elsewhere in the whole “NPZ” model, have been replaced with fixed values.

When we run the equations with the input values listed in Table 13.2, ensuring to test only one parameter at a time, and calculate the result values of S (from Eq. 13.1), we obtain the values shown in Tables 13.3 and 13.4.

| Configuration | | | | | | | |
|--------------------|--------------------|-------------------------|--------------------------|-------------|-------------|------------|------------|
| <i>mix_dep_fix</i> | 50 | | | | | | |
| <i>PFD_fix</i> | 1000 | | | | | | |
| <i>N_fix</i> | 2 | | | | | | |
| <i>P_fix</i> | 0.5 | | | | | | |
| <i>psq (Rn)</i> | 0.345 | | | | | | |
| Variable | Nominal value (Pn) | Low altered value (Pa1) | High altered value (Pa2) | Ra with Pa1 | Ra with Pa2 | S with Pa1 | S with Pa2 |
| <i>alpha</i> | 3.00E-06 | 1.50E-06 | 7.00E-06 | 0.294 | 0.383 | 0.30 | 0.08 |
| <i>ChlC</i> | 0.03 | 0.015 | 0.07 | 0.351 | 0.273 | -0.03 | -0.16 |
| <i>NC</i> | 0.1 | 0.05 | 0.2 | 0.248 | 0.383 | 0.56 | 0.11 |
| <i>Pmax</i> | 0.5 | 0.25 | 1 | 0.189 | 0.589 | 0.90 | 0.71 |
| <i>phy_k</i> | 0.5 | 0.25 | 1 | 0.376 | 0.296 | -0.18 | -0.14 |

Table 13.3 Sensitivity test configurations and results (S, Eq.13.1) for a high nutrient low biomass scenario with respect to *PSqz*.

| Configuration | | | | | | | |
|--------------------|--------------------|-------------------------|--------------------------|-------------|-------------|------------|------------|
| <i>mix_dep_fix</i> | 50 | | | | | | |
| <i>PFD_fix</i> | 1000 | | | | | | |
| <i>N_fix</i> | 0.5 | | | | | | |
| <i>P_fix</i> | 2 | | | | | | |
| <i>psq (Rn)</i> | 0.103 | | | | | | |
| Variable | Nominal value (Pn) | Low altered value (Pa1) | High altered value (Pa2) | Ra with Pa1 | Ra with Pa2 | S with Pa1 | S with Pa2 |
| <i>alpha</i> | 3.00E-06 | 1.50E-06 | 7.00E-06 | 0.086 | 0.124 | 0.33 | 0.15 |
| <i>ChlC</i> | 0.03 | 0.015 | 0.07 | 0.146 | 0.059 | -0.83 | -0.32 |
| <i>NC</i> | 0.1 | 0.05 | 0.2 | 0.056 | 0.174 | 0.91 | 0.69 |
| <i>Pmax</i> | 0.5 | 0.25 | 1 | 0.060 | 0.172 | 0.83 | 0.67 |
| <i>phy_k</i> | 0.5 | 0.25 | 1 | 0.128 | 0.075 | -0.49 | -0.27 |

Table 13.4 Sensitivity test configurations and results (S, Eq.13.1) for a low nutrient high biomass scenario with respect to *PSqz*.

These results indicate the following:

- Changes in $PSqz$ are positively related to α , with moderate sensitivity (i.e. $-0.5 < S < 1$). This is because the value of α directly affects the conversion of light into photosynthesis, by altering the slope of the PE curve (see Chapter 8).
- Changes in $PSqz$ are negatively related to $ChlC$, with moderate sensitivity (i.e. $-0.5 < S < 1$). The explanation for this is interesting. Increasing the value of $ChlC$ increases the rate of photosynthesis for the individual cell; this can be explored by manipulation of the Smith equation in Chapter 8. However, this does not help the collective population because the increased pigment load of the whole population decreases the amount of light, and hence depresses the growth rate. It is for this reason that for the commercial growth of microalgae genetic modification to restrict the highest value of Chl:C benefits biomass production (Kenny & Flynn 2015).
- Changes in $PSqz$ are positively related to NC , with moderate sensitivity (i.e. $-0.5 < S < 1$). In this model NC is linked to the calculation of the light absorbance (see Chapter 8). Coincidentally (and fortuitously), however, a high N:C in phytoplankton cells enables a high growth rate, while a low N:C (as seen in N-limited cells) is associated with a low growth rate. This is explored further in Chapter 15.
- Changes in $PSqz$ are positively related to $Pmax$, with moderate sensitivity (i.e. $-0.5 < S < 1$). This is expected as $Pmax$ directly controls $PSqz$.
- Changes in $PSqz$ are negatively related to phy_k , with moderate sensitivity (i.e. $-0.5 < S < 1$). This is because a low phy_k enhances nutrient uptake potential at low nutrient concentrations.

Note that this sensitivity analysis indicates the direction of the sensitivity for each parameter.

13.3 Things to explore using Single Parameter Sensitivity Analysis

- Does the sensitivity of any of the components of the phytoplankton model give you cause for concern? Which parameter (constant) affects growth rate most?
- Conduct a similar sensitivity analysis on the zooplankton model. In this instance you need to fix the value of P (phytoplankton) as a constant, by analogy to the selection of a value for N relative to phy_k mentioned above. The test parameters values are K_pred , G_max , AE and ex_rate .

13.4 Dynamic Sensitivity Analysis

While it is easy, if tedious, to conduct a steady-state single parameter sensitivity analysis, and this step should always be conducted on new model structures, things get more interesting and arguably more useful when conducting a dynamic sensitivity analysis. This is especially so when considering a combinations of parameter values, because of the cyclic interactions that may often ensue.

First we need to consider just how this analysis is conducted, and what mathematical or software approaches are needed.

The concept is simple:

- a) Each parameter value of interest is randomly varied (Monte Carlo –style) around a stated mean value (which may be the value fixed during “tuning” – see Chapter 14), by a stated standard deviation (SD) assuming a Normal distribution. If the SD is not known from empirical evidence (which is more than likely), then it can be set at a consistent value, such as 10% of the mean value. However, care must be taken not to set options for SD that would allow a variable to assume an impossible value. Thus, in consideration of assimilation efficiency for N (*AE*), the values must be between 0 and 1, and in reality would likely be between 0.1 and 0.9; here the randomly selected distribution needs to be truncated such that the test value is always within acceptable bounds.
- b) Having randomly selected the values for all the parameters being subjected to the analysis, the model is run and the output data for the processes of interest stored.
- c) Steps (a) and (b) are repeated a sufficient number of times to generate a total database covering the spread of outputs. The number of iterations depends on the randomising routine. The Latin Hypercube routine requires ca. $1/3^{\text{rd}}$ of the number of iterations needed for a traditional Monte Carlo routine, but even so we need 50+, and perhaps 100s of simulations in total.
- d) The statistical distribution of the output data at each time-step is computed (e.g., mean, SD, confidence limits), and these are plotted against time.

If all of this appears daunting then indeed it would be if you do not have access to software that does this all automatically for you. Assuming you do have such access, then all you then have to do is identify the test parameters, set the details for the randomisation process, select the output data types of interest, hit the button and wait for the many dozens of simulations to be completed, and then check the results.

In the following pages are presented the so-called “risk analyses” as performed by routines operated by the Powersim software. The plots show the sensitivities for individual parameters, and also for combinations.

The results are, in some instances, quite startling. For example, note the sensitivity to *AE* (Fig. 13.10), and then recall that this parameter is known not to be constant in reality, and hence there would naturally be considerable variability in its value and in outputs.

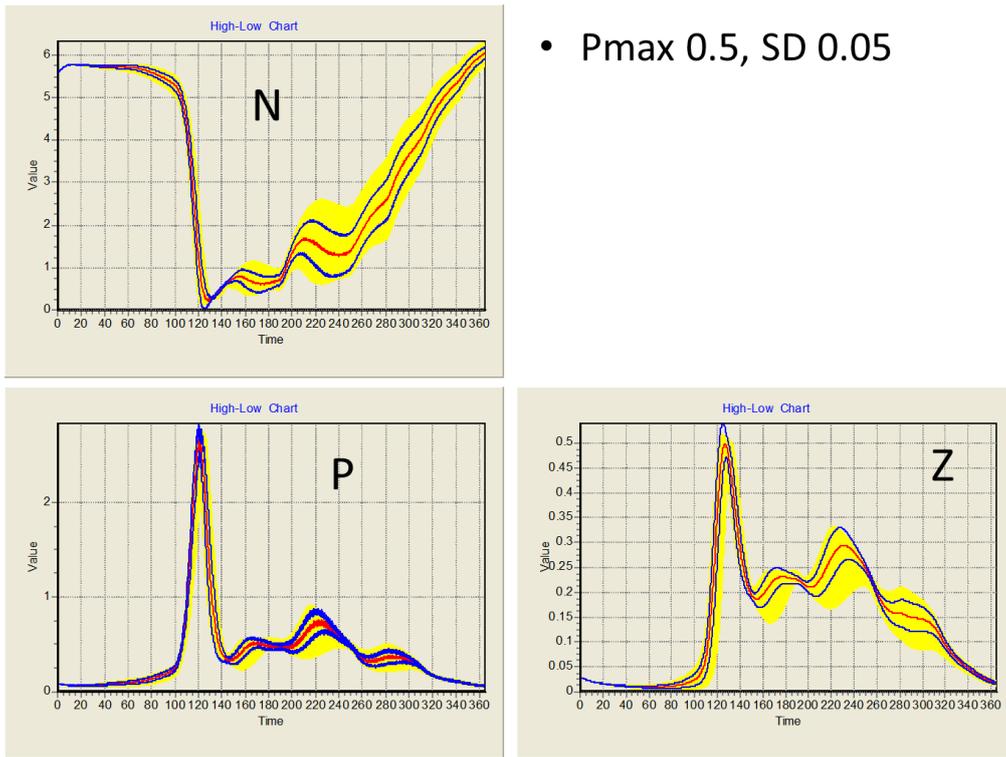


Fig. 13.2 Dynamic sensitivity analysis for P_{max} with the mean and standard deviation (SD) shown. Outputs are for nutrient (N), phytoplankton (P), zooplankton (Z) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

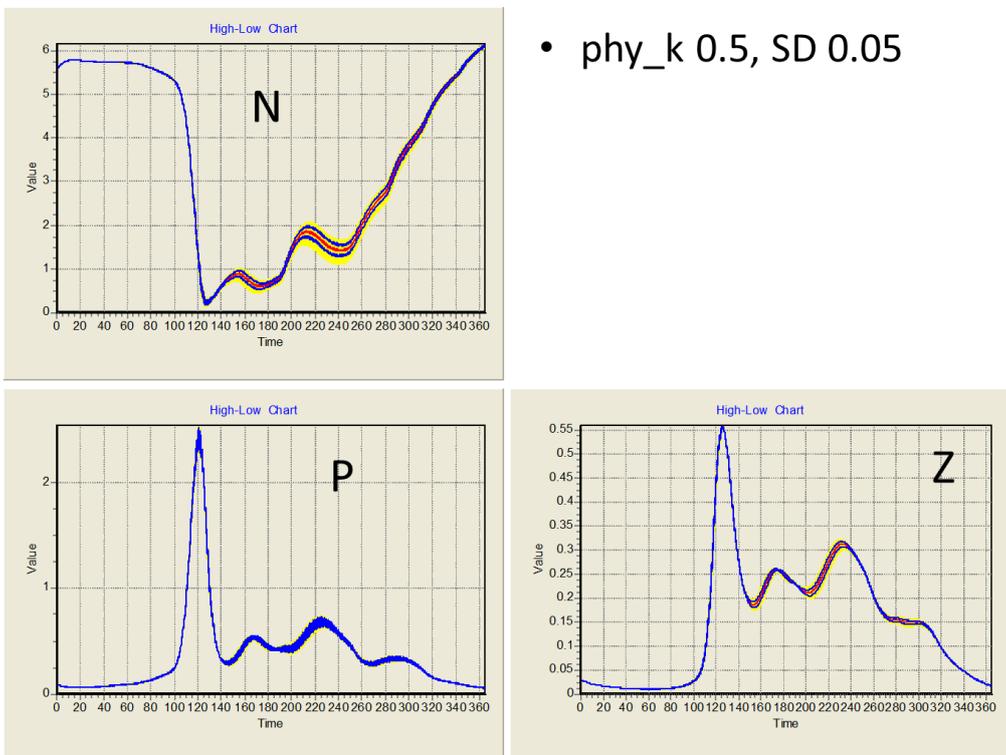


Fig. 13.3 Dynamic sensitivity analysis for phy_k with the mean and standard deviation (SD) shown. Outputs are for nutrient (N), phytoplankton (P), zooplankton (Z) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

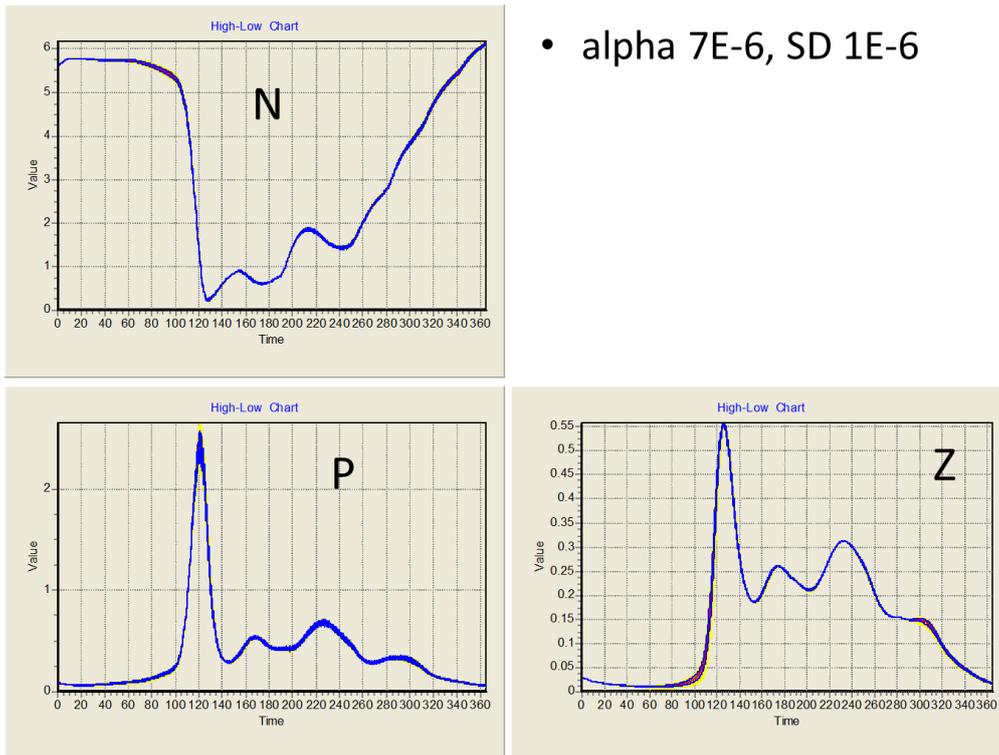


Fig. 13.4 Dynamic sensitivity analysis for *alpha* with the mean and standard deviation (SD) shown. Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

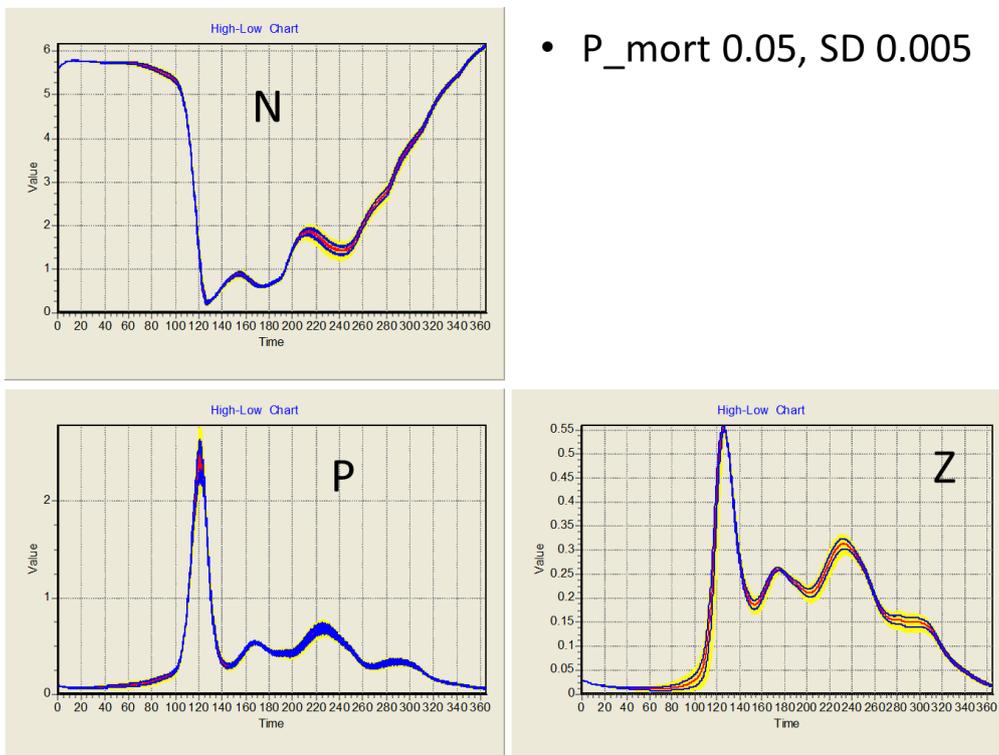


Fig. 13.5 Dynamic sensitivity analysis for P_{mort} with the mean and standard deviation (SD) shown. Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

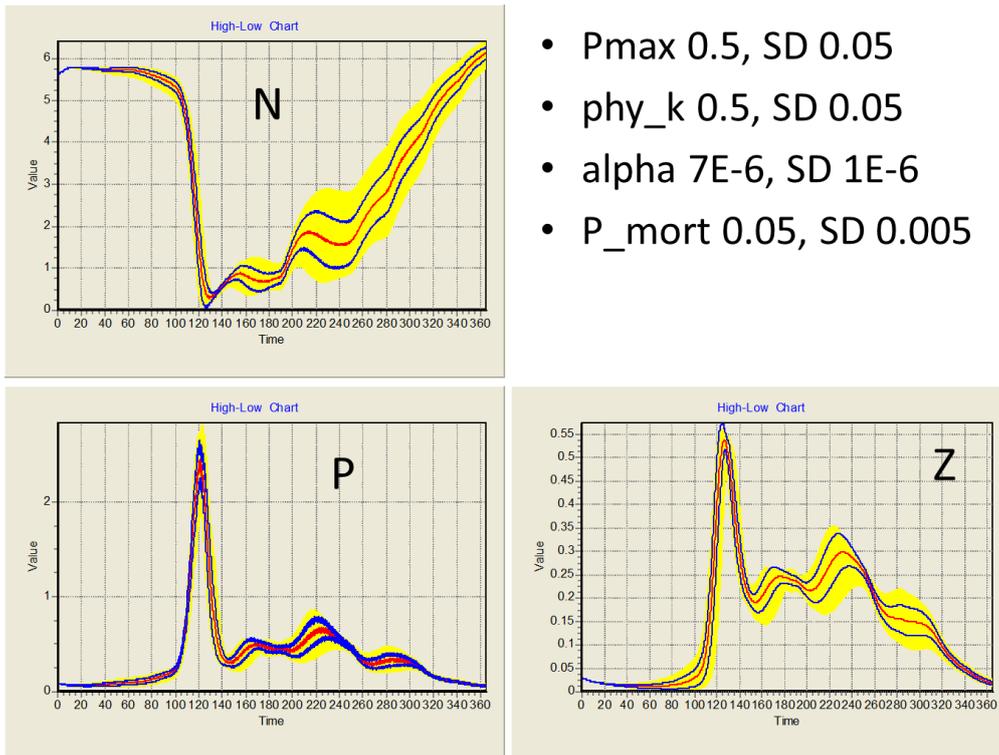


Fig. 13.6 Dynamic sensitivity analysis for the parameters stated with mean and standard deviation (SD). Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

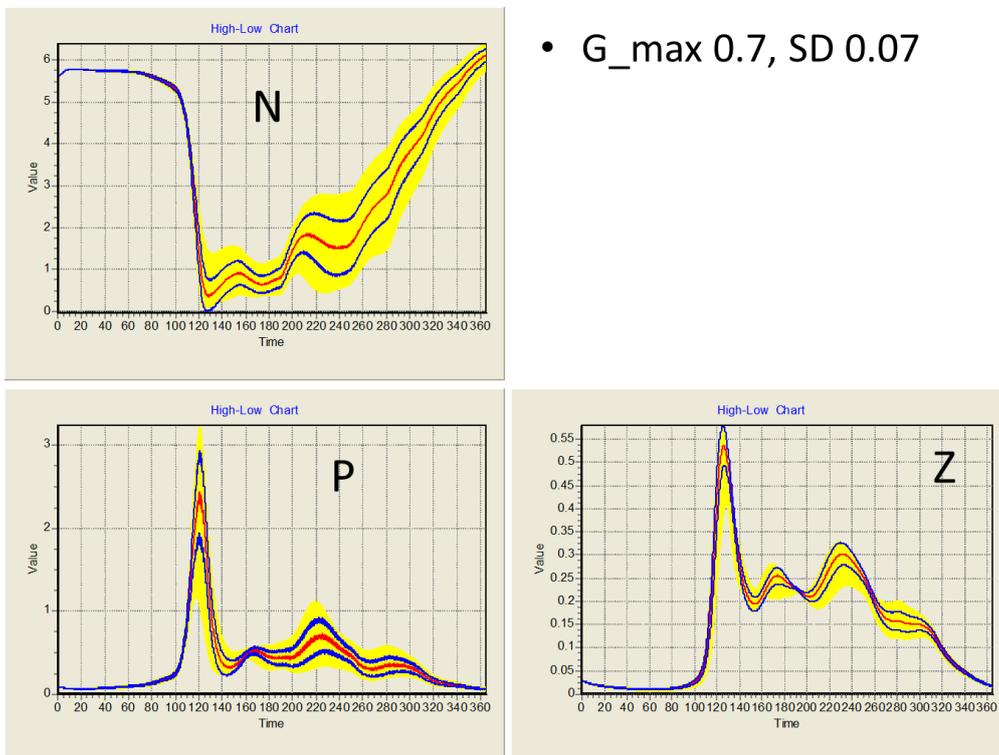


Fig. 13.7 Dynamic sensitivity analysis for *G_max* with the mean and standard deviation (SD) shown. Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

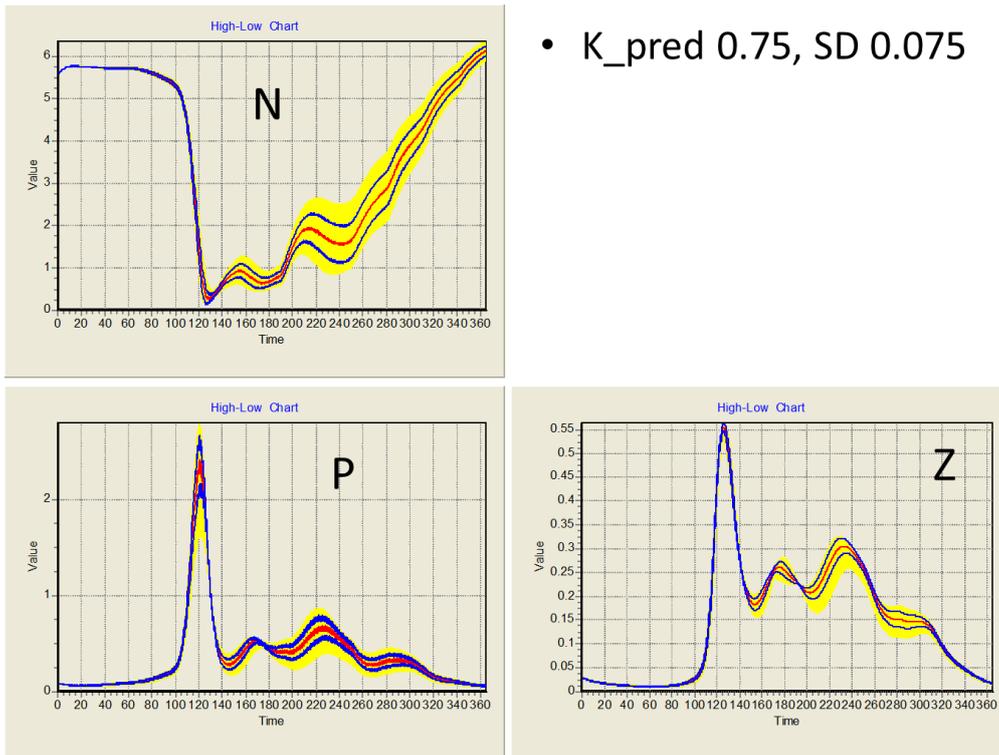


Fig. 13.8 Dynamic sensitivity analysis for K_{pred} with the mean and standard deviation (SD) shown. Outputs are for nutrient (N), phytoplankton (P), zooplankton (Z) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

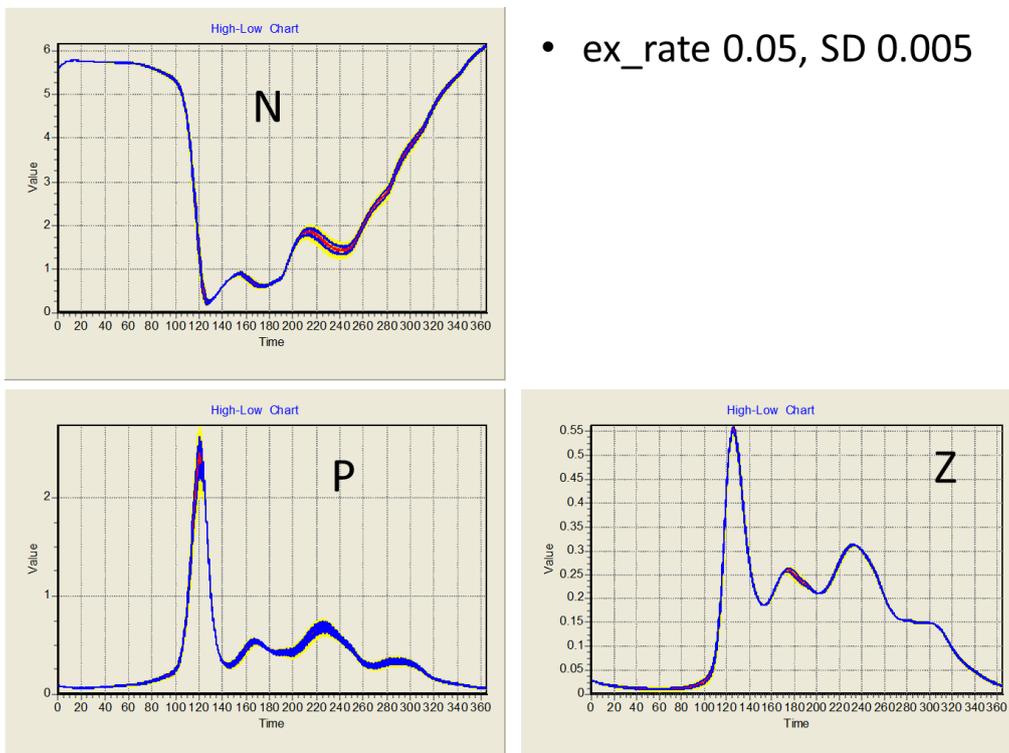


Fig. 13.9 Dynamic sensitivity analysis for ex_rate with the mean and standard deviation (SD) shown. Outputs are for nutrient (N), phytoplankton (P), zooplankton (Z) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

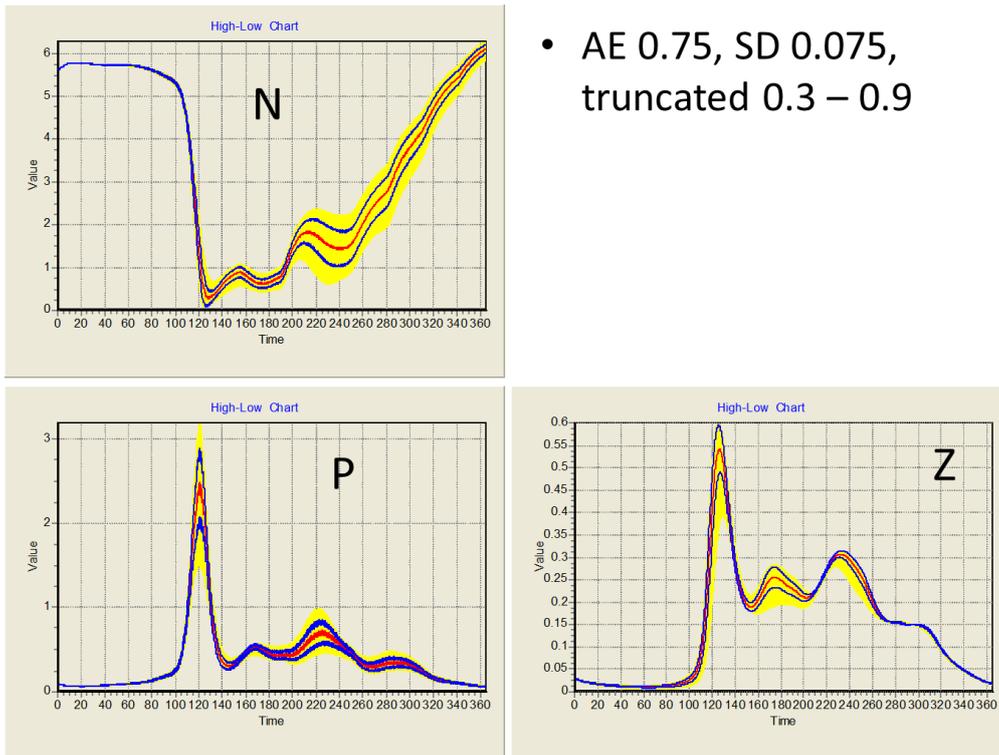


Fig. 13.10 Dynamic sensitivity analysis for *AE* with the mean and standard deviation (SD) shown. Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

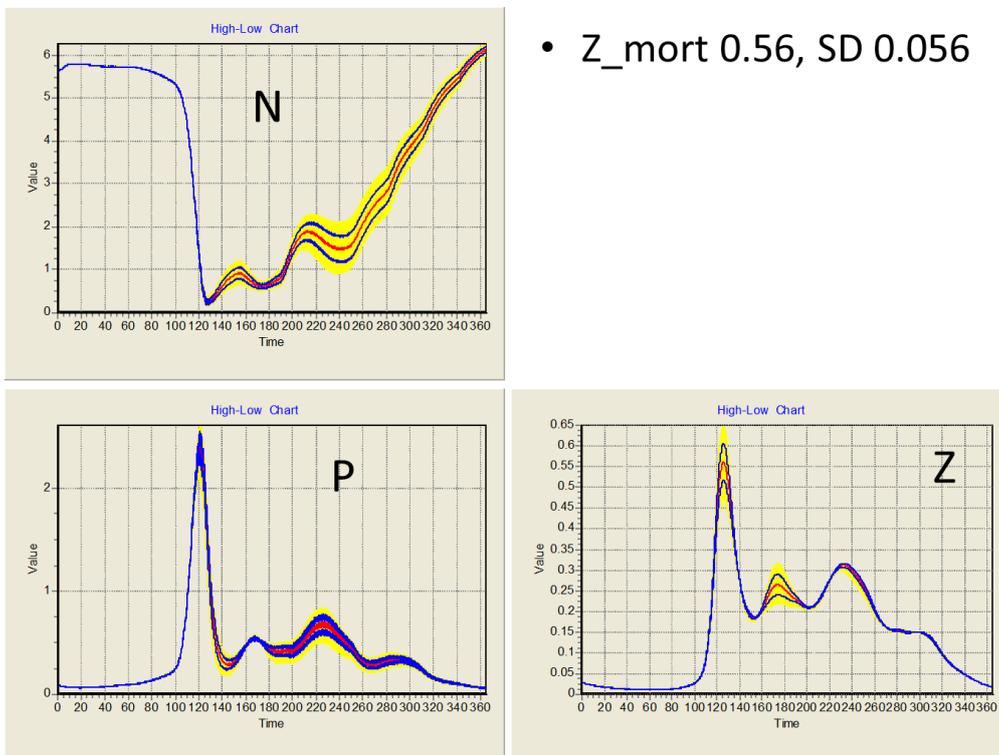


Fig. 13.11 Dynamic sensitivity analysis for *Z_mort* with the mean and standard deviation (SD) shown. Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

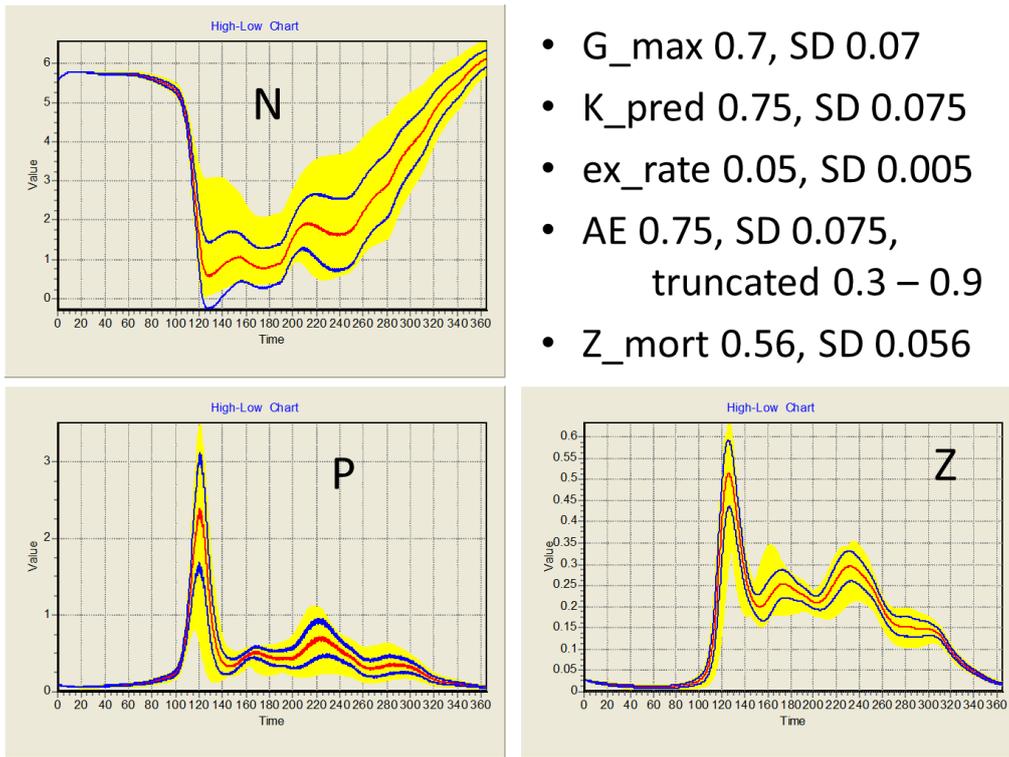


Fig. 13.12 Dynamic sensitivity analysis for the parameters stated with mean and standard deviation (SD). Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

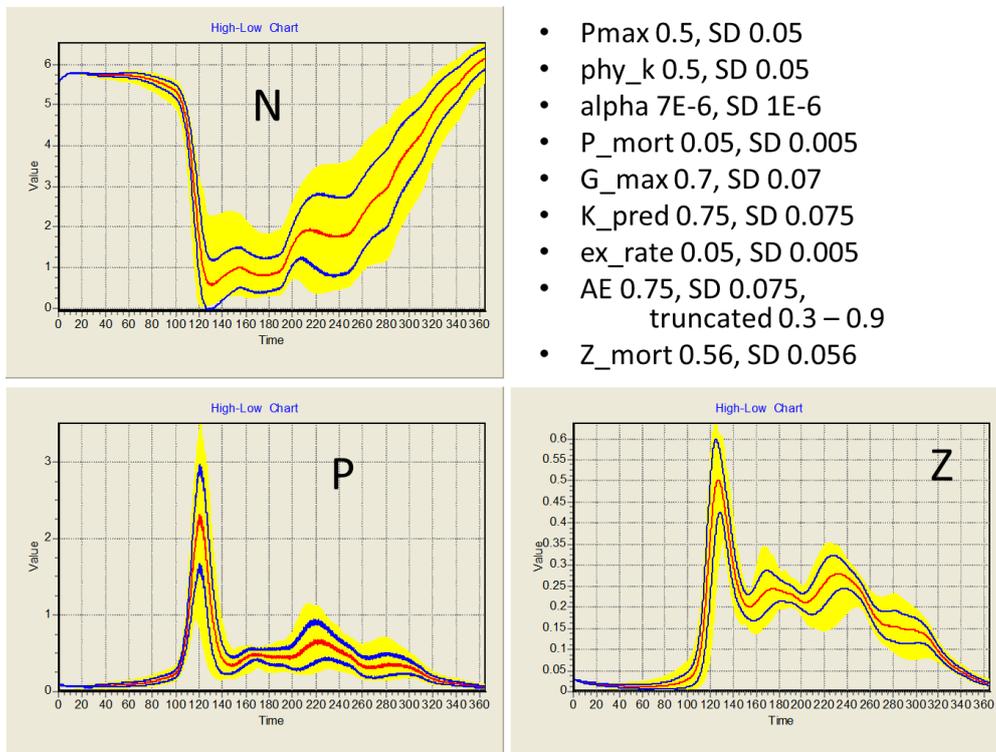


Fig. 13.13 Dynamic sensitivity analysis for the parameters stated with mean and standard deviation (SD). Outputs are for nutrient (*N*), phytoplankton (*P*), zooplankton (*Z*) showing mean (red) SD (blue) and 95% confidence limits (yellow fill).

13.5 Things to explore with Dynamic Sensitivity Analysis

- i) Compare the results of the dynamic sensitivity analyses with those from the steady-state single parameter analyses. Consider the usefulness of the information provided by each approach.
- ii) Seasonality, and allied factors, may be expected to have a big effect on the behaviour of any simulation linked to the weather and/or climate, such as the “NPZ” model. While the seasonality of the sunlight profile is fixed (though cloud cover is not), an “early” spring may result in the shallowing of the mixed layer depth earlier in the year when there is less light from the sun. Conversely, a “late” spring would shift the timing of the spring bloom to a time of greater daily irradiance. One way to explore the implications of this would be to create a constant defining a “seasonal offset”; this would need to shift the reading of the *mix_depth* and *H* by a period either side of the value of *JD*.
- iii) Cloudiness is another factor one may well expect to affect primary production. The sensitivity of model behaviour to the value of *atmos_clar* in the light module (see Chapter 9), which is held constant in the “NPZ” model (Chapter 12), could also be explored.
- iv) Consider what these analyses tell you about the importance of empirical data, and also of the reliability of models as predictive tools.

13.6 Where Next

Sensitivity analyses should be conducted around a midpoint, default value for each constant parameter. In some instances that value may be well established, but often there is a need to optimise or tune the model fit to real data. Chapter 14 considers how to achieve such an optimisation.

14. Tuning (Optimising the Fit) to Data and Validation

Terms and concepts introduced in this chapter- tuning, optimisation, evolutionary searching, data quality, weighting, validation, skill

14.1 Ecological Context

To have any confidence in your simulations, such that you could operate your model in a predictive fashion, you need to compare the outputs to reality and then consider whether you think that fit is sufficiently convincing. To optimise the relationship between your model's behaviour and reality, you need to select values for input variables (constants) that best equip the model to follow the expected patterns in output. Here we consider the mechanics of adjusting the values of the constants controlling how the equations work so that the outputs conform as closely as possible to a real data series.

This process is termed by some as “optimisation” (of the model output to a truthing test data series), while others term it “tuning”. Some use the word “training”.

Some confusion can occur because “optimisation” is also used in the context of commercial applications where a model is run with different values for inputs until some target is attained (e.g., maximising productivity while minimising financial outlay). The target for optimisation in such a context is typically judged at the end of the simulation (akin to the end-of-year balance sheet of a company). From hereon we will use “tuning” to identify a process of matching the temporal output of a model to truthing data. In some ways the mathematics are similar; in “tuning” you are trying to “optimise” the fit to data by minimising the difference between model output and externally provided data.

Tuning involves a comparisons between model output over the duration of the simulation with data; in automated tuning (optimisation, if you wish) the target is to minimise the cumulative sums of squares of the differences between the model output versus test data over a time series.

Deciding whether your model fit to the data is convincing can be highly subjective. Some parts of the output may be a better fit than others, for example. To help you in this judgement, you should undertake a validation step, in which you compare model output against a different data set to the one you used for tuning, but with different forcings (e.g., different nutrient levels, different mixing depths). Validation is considered at the end of this chapter.

14.2 Automated vs Manual Tuning

Working manually, the process of tuning would involve the sequential alteration of each constant, the running of the model and then some method of comparing model output to “reality”. The human eye is actually very good at the latter process and the brain also imparts a level of common-sense to curve fitting (ignoring outliers), but the mechanics of the alterations themselves can be extremely time consuming. That is especially so with models of higher structural complexity.

A solution is to use a system that randomly trials potential values for each constant, runs the model and collects the cumulative sums-of-squares deviations between “simulation and truth”. Eventually, after an extremely high number of alternatives have been trialled, the best options would be selected. But there is an even better way than this, as we shall see below.

14.3 Tuning Using an Evolutionary Search Method

Instead of randomly assigning values to the constants, the evolutionary approach keeps a track of values for each trialled constant that is associated with a relatively good fit. Subsequent trials avoid values of constants that give poor fits. The system thus “learns”; it evolves through selecting the best combinations of options.

There is a danger, however, and that is of locating what is termed a **local minimum**. This event occurs when a combination of input (constant) values give a small deviation between model output and the truthing data, such that altering the constant values a little either side actually increases the deviation. The automated system could become trapped here, unaware (so to speak) that a better fit exists at a different combination of constant values. To escape from this trap the program uses another feature of evolution, that of mutation. Randomly, alternative values (mutations) are thrown in to test whether a lower minimum (a better optimisation to the fit) exists away from what could be a local minimum.

14.4 Evolutionary Tuning in Action

Below we consider the tuning of the “NPZ” model (Chapter 12) against real data collected from an oceanographic study. The process is demonstrated using the genetic evolutionary procedure supported by the “tuning” component of the Powersim Constructor / Solver platform. At the time of writing this is not available on the successor to Constructor (Powersim Studio); however, “optimization” is available and you could readily configure a sub-model to provide a cumulative sums-of-squares-of-deviations between model output and data series, using the “optimize” tool to identify values for constants that minimise those sums-of-squares. Other platforms have tools of different abilities; it is worth checking them out.

The process operates through the following steps:

- i) Identify the constants that are to be tuned (e.g., maximum growth rates), their current values (which, at the least, enable the model to run in a plausible fashion), and the extremes of the plausible range of values that each constant could take.
- ii) Locate suitable data series to act as the “truth” data. These may likely need to be transformed to provide numeric values in the appropriate units. It should be noted that these transforms (such as converting cell biovolume in to N-biomass units) themselves often represent major sources of error in the whole process. The failure of a model to match data need not necessarily be solely down to problems with the model; the failure could very often in part reflect problems manifest in the original data and/or with the experiments used for their collection. Indeed, one of the important reasons to train biologists to undertake modelling is because it generates scientists who are more aware of

- the types of data required for modelling. In the context of our “NPZ” model, the paucity of reliable zooplankton data represents something of an Achilles Heel, as we shall see below.
- iii) Check through the “truth” data series, rejecting values that appear as outliers. It may also be necessary to use some level of judgement to add additional data points to the truth data series. Why? – is this not “cheating”? Well, no, not really. It is highly likely that a time-based data series will be patchy; for the data series we will use below there are large periods of the year for which there are no data at all – most effort in oceanographic cruises is expended studying events such as the spring bloom, with studies in the winter and even the mid-summer being rare. However, from other sources of information it is quite likely that you will have a good feel for what is happening in these data-poor zones. Remember what you are trying to do here is provide a framework for guiding the tuning process. Another thing to remember is that you are most likely trying to obtain a model that describes generality; typically you will not know if the data set you do have access to is really even representative of every year, so there is little sense in getting overly concerned over every data point.
 - iv) Some types of truth data will be more reliable than others; estimates of rate processes for example are likely to be far less reliable than measurements of abundance or concentration. In addition, invariably some of the numeric ranges will be very different to others; thus nutrient biomass may range from 0 to 100 μM , while Chl:C will range from ca. 0.01 to 0.07. Why is this important? The target of the tune is to minimise the sums of squares of the deviations between model output and the truth data; deviations associated with data that have large numeric values will thus exert greater leverage on the tuning process. Reference to data series of low numeric value and those which are of greater reliability may need to be **weighted**, so that the tuning process evolves by taking more note of getting the fit to these “more important” data types than it would otherwise do.
 - v) The information gathered so far are used to inform the programme. The final step is to configure the rules of the generic evolutionary algorithm. The more constants that are being subjected to tuning the larger the “family” of options needs to be for selection; this also means that each generation will take longer to simulate.
 - vi) For the example at hand, the “NPZ” model described in Chapter 12, each simulation needs to run over several years, not just the one year plotted in Chapter 12. This is because it takes some time for the model to “spin up”. For complex 3D basin-wide or global simulations this spin-up can take the equivalent of many decades because it takes so long for cyclic processes involving water currents to enter a quasi-steady-state. Indeed, for these reasons, these complex models are not usually tuned as such. For the simple model used here it is sufficient to run the model over a simulation period of 3 years.
 - vii) The programme is now run over hundreds of generations, with each generation running 10, 20, 30 or so combinations of parameter constants (so in total 1000s of simulations are performed). The software takes the best of each generational run and “crosses them” (in the style of genetic recombination) to inform the programme of the best options for the next generation. Eventually the numeric mismatch of the simulation outputs and the truth data falls to acceptable levels; the values of the input constants for that final simulation are taken as those providing the optimal, tuned, fit. Of course, even after all of this the fit may not be good at all. In that instance you need to double check all the above steps, and then the conceptual basis of your model.

The tune data for the “NPZ” model running at the NABE oceanographic station are shown in Fig. 14.1. The model is already configured with the appropriate values of *mix_dep*, latitude (*lat*)

and atmospheric clarity (*atmos_clar*). Values for the constants to be tuned are given in Table 14.1, together with the selection window of values for their tuning.

| Input Variable (constant) | Initial value | Window of values used for tuning | Final tuned value |
|---------------------------|---------------|----------------------------------|-------------------|
| <i>AE</i> | 0.8 | 0.5 - 0.8 | 0.75 |
| <i>alpha</i> | 1.46E-06 | 1E-6 - 8E-6 | 7.00E-06 |
| <i>ChlC</i> | 0.054 | 0.02 - 0.06 | 0.06 |
| <i>ext_NO3</i> | 6.686 | 5 - 8 | 7.25 |
| <i>G_max</i> | 0.64 | 0.5 - 1 | 0.7 |
| <i>initN</i> | 6.446 | 4 - 8 | 5.6 |
| <i>K_pred</i> | 1.38 | 0.5 - 1.5 | 0.76 |
| <i>NC</i> | 0.105 | 0.1 - 0.2 | 0.15 |
| <i>P_mort</i> | 0.0237 | 0 - 0.1 | 0.05 |
| <i>phy_k</i> | 0.2 | 0.2 - 1.0 | 0.5 |
| <i>Pmax</i> | 0.3 | 0.3 - 1 | 0.5 |
| <i>remin_frac</i> | 0.096 | 0.05 - 0.8 | 0.167 |
| <i>Z_mort</i> | 0.5 | 0.5 - 1.5 | 0.56 |

Table 14.1 Variables (constants) subjected to tuning, their initial values, the selection window of values used by the tuning process, and the final values that gave the best fit to the data according to the evolutionary algorithm deployed.

| Output Variable | Weight | Initial deviation | Final deviation |
|-----------------|--------|-------------------|-----------------|
| <i>N</i> | 1 | 0.784 | 0.289 |
| <i>P</i> | 2 | 0.549 | 0.105 |
| <i>Z</i> | 100 | 0.01726 | 0.0056 |
| Total | | 3.6 | 1.059 |

Table 14.2 Weightings applied for tuning of model output for *N*, *P* and *Z* against tuning data, the initial deviations between model output and the corresponding data series (see Fig. 14.1) and the final deviations. See also Fig. 14.2. Note that the total deviations take into account the weight assigned to each parameter.

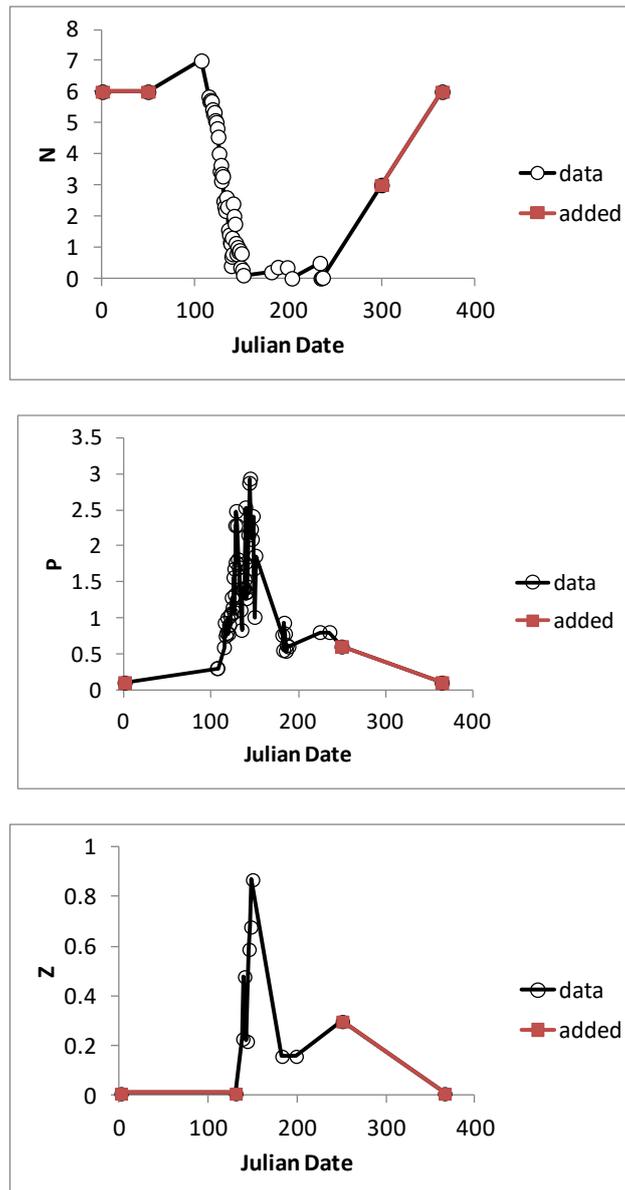


Fig. 14.1 Data used for tuning the NPZ model. Indicated are those data points originating from real observations, and also those added based on phenomenological expectations by the author.

The tuning algorithm is then put into action. Fig. 14.2 shows how the deviations between the model output and the data series used for truthing change during the process. Note that while the total deviation decreases over time this is achieved on occasion at the expense of some components actually becoming worse fits. Thus, each of the N , P and Z deviation plots show periods of increases in deviations. What is happening is that the evolutionary algorithm is trading off some advantages against others to improve the overall fit of the model. The importance of weighting the zooplankton data series heavily now becomes apparent; if this is not done then a really good fit is achieved for N and P but with a really bad fit for Z .

It is important during the process to keep an eye on what values are being evolved for each of the constants. If these values run up against the upper or lower extremes of the selection window specified at the start of the process (step #1, above; Table 14.1), then it may be necessary to re-run the process with the window widened. Care should be taken in doing so not to exceed plausible values for each constant type.

The final fits of the model are given in Figs. 14.3; in general terms it can be seen that the model output fits the data used for truthing quite convincingly.

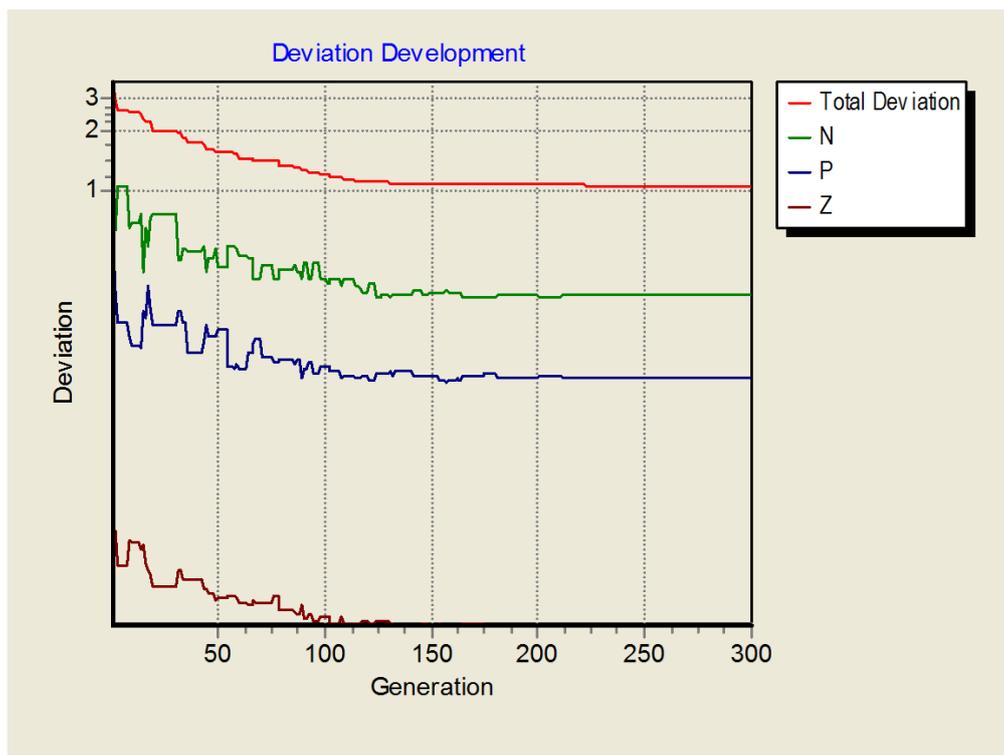


Fig. 14.2 Plot showing changes in the deviations between model output and the truthing data series. The value of the Total Deviation takes into account the weighting applied to the deviations for Z (weight=100) and P (weight=2), with N (weight=1); see Table 14.2. Note that while Total Deviation always declines this is on occasion achieved through an improvement of some fits (decreased deviation) set against a deterioration (increased deviation) of others. The Deviation axis is a log scale.



Fig. 14.3 The final fit of model output (N , P or Z) versus their corresponding data series (see also Fig. 14.1). Note the simulation is run over 3 year cycles, with the fit improving in years 2 and 3 once spin-up is achieved.

14.5 Things to Explore with Tuning

- i) Revisit the issues of sensitivity of the model to parameter values, and also to the effects of changes in seasonal-related factors (see Section 13.4), questioning how much emphasis should be placed on a fit to empirical data collected during just one year.
- ii) Consider whether it would be better to run a tuning process as here, against a continual “truth” data series with involvement of what one may describe as phenomenological data (insight) to plug the gaps in the empirical data, OR strictly against only the empirical data points at those few times when they were collected.

14.6 Validation

Optimising a model to best represent the processes of interest is a complicated topic from many angles. Perhaps the most important single issue is simply the availability of appropriate data to not only tune the model, but to then run a validation exercise.

For validation the tuned model is run against a new data series, with no constants changed except for any site-specific values, and a judgement made upon whether the model describes the situation to the satisfaction of the researcher. Here, for example, the same ecological model tuned for NABE could be run against physics for a region in the Pacific.

It is notable that there is a great deal of subjectivity in all of this. While some objectivity can be applied to judging whether one model fits data better or worse than an alternative model, judging whether either is “good enough” can certainly be highly subjective. It is more so if some outputs fit data well, while other diverge from them. Which data are of greater importance to you? Are you more or less concerned about the timing, or of the magnitude of the events? The least that can be done is to identify and then remove dysfunctionality (Section 6.9), to prevent the model describing events that simply do not occur in the real world (Flynn 2005a, 2010).

Unfortunately, all too often (especially for field studies), all the available data are used for tuning and none remain for validation. For laboratory studies, at least repeating the data collection exercise is possible, provided the facilities are still up and running. And this rather speaks to the importance of properly integrating modelling and data collection within a project. Too often modelling comes at the end of a project, where there is no capacity to repeat experiments or collect more data or different types of data.

14.7 Model Skill

Skill is a term used to describe how well a model output agrees with reality; it provides a metric for comparing the performance of different models. The simplest metric is the Pearson correlation coefficient calculated between real and modelled (simulated) data. Comparisons between a few models can be made using tabulated statistics. However, more complex data series and comparisons between many models generate many statistics and require visualisation; this may be undertaken using a **Taylor diagram**.

None of this takes away the subjectivity of deciding whether a good fit for one parameter justifies a poor fit for another, as mentioned in Section 14.6. However, it does at least give a platform to

provide (perhaps) some objectivity for the subjectivity. At the back of all these comparisons is the question of how good, how representative, is the “real” data series that provides the benchmark.

14.8 Where Next

The issue of data availability is typically viewed in the context of numeric data. The alternative is to consider the use of non-parametric data and “expert witnesses”; in essence get an expert in ecology to test your model behaviour for you. This route enables you to provide more objectivity to the whole process. The other important role for such experts is to guide you in identifying the best numeric data against which to configure your model. Many values for key parameters (such as growth rates, assimilation efficiencies etc.) in the literature are questionable and it can take a real expert to guide you through the maze. Data may be questionable for various reasons, but a common one is simply because science has moved on and techniques and interpretations have changed. That “classic paper” may not be the font of all knowledge that you may think it is as gauged from the high citation record.

15. Variable Stoichiometry – a Simple C:N-based Phytoplankton Model

Terms and concepts introduced in this chapter- stoichiometric ratios, multi-currency, differential or variable stoichiometry, ecological stoichiometry, Redfield ratio, quota-control of growth, cell-quota, Droop

15.1 Ecological Context

Hitherto we have considered simple, single-currency, models. In all instances we have used N as the currency, and hence described all ecological interactions with respect to the transfer of that element. We could have used P instead of N, but of course in real systems many elements, and indeed many biochemicals (notably so-called essential amino and fatty acids) are transferred and that transference could be rate limiting for growth. Most obviously C (for both structure and energy) is transferred.

The ratio of different elements and of biochemicals to each other differs between organisms, and also within organisms of different physiological status. Such ratios are termed **stoichiometric ratios**. In consequence of differences in stoichiometry, during trophic interactions there is scope for interactions developing because of an excess in one component (element or biochemical) in the food versus that in the consumer. This excess needs to be removed. The flip side is a shortage in one or other components that causes an inadequacy in the nutritional value of the diet.

Models that describe the resultant interactions of differences in chemical composition are **multi-currency**, exhibit **differential stoichiometry**, and usually (in reflection of changes in stoichiometry in the individual organism depending on their nutrient history) they are **variable stoichiometric**. Thus, for example, they describe variations in C:N:P in each organism functional type during trophic interactions. In much of ecological research, while it becomes very obvious (as we shall see in this chapter and in Chapter 16) when operating variable stoichiometric models that such variability has profound impacts on the dynamics of ecology, it took the advent of the now classic work of Sterner & Elser (2002) on “**Ecological Stoichiometry**” to bring this matter to the attention of mainstream ecology.

In marine biology and oceanography the importance of such matters has been suppressed by the advantages of assuming fixed, invariant stoichiometry according to the Redfield ratio (Redfield 1958). The Redfield ratio has been used to assume an average fixed mole C:N:P of 106:16:1 (mass ratio 41:7.2:1) in marine plankton. The Redfield ratio represents something of a cornerstone concept in biological and chemical oceanography. It simply reflects empirical observations concerning the typical ratio of these elements in particulate material collected across the world's oceans. Although some suggest a biochemical basis for such a ratio, in fact there appears to be none (Geider & LaRoche 2002). Ironically, the basis for modelling variable stoichiometry was developed not that long after Redfield's 1958 paper, by the work of Droop (1968) upon marine phytoplankton.

In this chapter, and the next, we commence a consideration of the challenge in modelling variable stoichiometry. Typically in our context this refers to elemental stoichiometry such as C:N:P within organic material (organisms, faecal material, dissolved organics); for simplicity we shall restrict our considerations here to C:N. We could also apply the concept to biochemical stoichiometric ratios

such as protein:carbohydrate, down to ratios of specific amino acids to protein, or PUFA to total fatty acids. In organisms these ratios vary within bounds depending on the physiology. The ratios are also bound by biochemistry; for example, the C:N in protein is constrained by the C:N in the constituent amino acids, and ultimately by the fundamentals of chemical valency.

15.2 Variable Stoichiometry

Stoichiometric ratios are particularly variable in primary producers, as these organisms balance incoming separate streams of C from photosynthesis and N and P from inorganic sources. In heterotrophs the ratios tend to be less variable as the nutrient streams into these organisms are of combined elements that are already constrained by the chemistry and biochemistry of the biomass of their prey and/or of organic nutrients. However, it is a technical fallacy to consider stoichiometry within and between heterotrophs to be invariant.

In every trophic interaction (except cannibalism perhaps) there is a difference between the stoichiometry of consumer and food (predator and prey, if applicable), so that some components are in excess and must be discarded. Respiration (removing C) also affects the ability to retain, and hence the need to discard excess (termed “regenerate”), N and P. These discards, as organic particulates or inorganic/organic dissolved materials, re-enter ecology elsewhere in the food web.

It is important to recognise that nutritional quality is far more than just that represented by elemental stoichiometry; the relationship between C:N:P and food quality cannot be considered as linear (Mitra & Flynn 2005). For example, when a phototroph is deprived of nutrients (notably when P-stressed) they not only increase the cellular C content (i.e., C:N and/or C:P increase) but often they synthesise more secondary metabolites, which may include noxious compounds, if not potent toxins. For this reason, quite minor changes in elemental stoichiometry may be associated with significant changes in quality that may result in the food being rejected or otherwise being suboptimal for a consumer. In turn this can have far reaching and potentially ultimately counter intuitive implications for the dynamics of ecology (Mitra & Flynn 2006a, 2006b).

15.3 The Challenge

The need to consider variable stoichiometry in simulations can be controversial. The major problem from a modelling perspective is that for each element an additional state variable is added. And this is so for every component in the system that has variable stoichiometry. For sure it is very convenient to assume a fixed stoichiometry such as that described by the Redfield ratio; you only need to track one element and the others follow automatically – hence the N-base of the “NPZ” model in Chapter 12.

And then there is the matter of data availability and indeed our phenomenological understanding of how all these stoichiometric interactions play out. Field ecologists have tended to emphasise control factors at the level of food acquisition (such as prey encounter rates, and prey handling) with rather little emphasis on food quality. In contrast, food scientists and nutritionists assume a saturating supply of food for acquisition and emphasise the importance of quality. In reality both quantity and quality of nutrition are critical determinants for an individual organism, and how an organism copes with these two factors is inter-dependant.

Returning to data availability, few researchers measure C:N:P, let alone C:Si or C:Fe. Carbon and N are usually measured together in CNH elemental analysis and the process is neither trivial nor inexpensive to undertake. Phosphorus and Si are less expensive to measure, but again not trivial. Iron requires special precautions to prevent contamination during sampling and analysis. Further, often with plankton communities it is not possible to separate different organism types, or indeed to separate organisms from faecal material.

There are, however, other routes to estimating the organism elemental content. Carbon content correlates well with organism volume, and so it can be estimated from measurements of size (Menden-Deuer & Lessard, 2000). Using this approach it may be possible to estimate at least the C-biomass allocation to different organisms. The content in terms of N, P and Si can be estimated in flask cultures from the consumption of inorganic nutrients; this however makes the important assumption that all that disappears from solution as the measured inorganic nutrient is captured within the organism of interest.

What we do know for sure is that only in very few instances will elemental stoichiometry be fixed in ecology, and that is even less likely when one considers trophic webs of any complexity. For applied (commercial) applications a consideration of variable stoichiometry is important as it affects the value of a crop; the content of a particular product (e.g., types of fatty acid, such as PUFA) varies with organism health, and this is reflected in changes in stoichiometry.

15.4 Modelling Variable Stoichiometry; the choice of state variable descriptions

Having established that modelling variable stoichiometry is useful if not of great importance, let us now consider the construction of a simple example of a nutrient-limited growth of a phytoplankton. Here we will consider that nutrient to be ammonium-N and we thus consider the variable stoichiometry of the phytoplankton in terms of C and N.

Firstly, we have a simple decision to make – are our state variables for the phytoplankton to be described as C (e.g., gC m^{-3}) and N (e.g., gN m^{-3}), or as C (e.g., gC m^{-3}) and N:C (gN gC^{-1})? The state variable count is the same, and both options include C as a currency, but the philosophy and pragmatic consequences behind the decision between using N versus N:C as the other state variable need to be reviewed.

Reasons for using N:C are :

- It emphasises (reminds the modeller) that N is inextricably linked to C within organisms and that N:C cannot deviate beyond certain bounds.
- In the context of biochemistry, of how the organism functions, the concentration of nitrogenous components relative to others (here as N:C) has a real meaning. It also has a real meaning for ecological stoichiometry.
- In the context of a food web, there is no need to describe trophic transfers in and out of the state variable; the value of N:C in phytoplankton is not affected directly by changes in phytoplankton abundance. If N was used as the state variable then a flow out of the phytoplankton N would be required in addition to that out of phytoplankton C.

Of course, it is easy enough to compute N:C from the values of state variables N and C, and at the end of the day one may argue that it makes little difference for modelling. But for biology, and we

are modelling biology, N:C at least means something while separating organism C and N appears artificial.

An example of a similar type of fundamental choice in model building could be seen in describing plankton biomass in a lake. The options are to have state variables for lake volume (m^3), and then either for biomass concentrations (gN m^{-3}) or for biomass abundance (gN). Which option would you use, why and when? (We constructed such a model in Chapter 10.)

There is, however, another important issue for application of biological models within ecosystem simulators that describe the movement of organisms between different bodies of water. Plankton are mainly moved passively by water currents, and are accordingly invariably treated as “passive tracers” in ecosystem models. That is to say that when, at each integration step, a portion of the water body in one gridded zone is exchanged with water in adjacent gridded zones, the dissolved nutrients, salinity etc. are also so-exchanged, and so also are the plankton. To undertake these calculations requires that the elements in the plankton are all *de facto* treated as passive tracers and are moved according to the same rules. It is not possible to undertake such exchanges with reference to state variables of elemental ratios, such as N:C.

There is a catch though. Running a model of plankton according to a passive tracer concept belies the fact that in reality these are not actually passive tracers at all. The organisms (as plankton) may indeed behave as passive tracers, but their contents certainly do not; the value of cell:C:N:P:Fe (etc.) is a function of non-passive regulations under complex biochemical control. If we mix two populations of different C:P the resultant population does not in reality recombine their C and P to achieve a new average C:P. This would be like mixing two populations of rich and poor individuals and expecting that the resultant population behaviour will reflect an equal distribution of wealth.

The ultimate solution would be to describe populations as agent-based using a (so-called) individual based model approach (see Section 2.9). Whole sub-populations would then be exchanged between zones. This raises the level of complexity massively. If we are happy to accept the relatively minor exchanges in passive tracers between adjacent zones undertaken at each time-step, and also assume that the ratio between the tracers within a given plankton group is also relatively minor, then we can live with the error in averaging two populations. Accordingly, it makes more sense to build models describing plankton as if they are composed of disjointed elements, with state variables as gC m^{-3} , gN m^{-3} , gChl m^{-3} , etc. Reference to ratios of components (as N:C, P:C etc.) is thus achieved via auxiliaries.

15.5 The Concept of Quota-Control of Growth

Using a variable stoichiometric model allows us to do more than just describe changes in stoichiometry. The physiological state of an organism affects, and is affected by, its stoichiometry. These relationships vary between organisms, and in some respects may appear diametrically opposed. Thus, for an animal the accumulation of excess C (as fat) could be taken to infer that the organism is fitter than one that contains no excess C; certainly that is so when the animal is confronted with periods of starvation. In phototrophs, however, an excess of C indicates above all else that C-fixation is out of balance with the acquisition of other nutrients. In fact, the internal availability of the limiting nutrient can usually be related directly to the potential growth rate. If you think about it, this makes sense; it is not the availability of food in the environment that

controls your growth, but the concentration of food inside you. Of course one is linked to the other, but as we shall see there are various consequences that stem from separating the events. This is an important concept and is one that is often termed something along the lines of the **quota-control of growth**. The “quota” in this context refers to the amount of a potentially limiting resource referenced to the organism as a whole. It provides a measure of the nutrient availability inside of the organism.

The concept of the quota-control of growth is typically ascribed to the **cell-quota** concept of Droop (1968), often also termed the **Droop-quota** concept (see Flynn 2008b). The cell quota describes the amount of a substance in a unicellular organism. The original application was towards vitamin B₁₂ per microalgal cell, but the concept has been expanded to P and then to N. The value of the quota governs how quickly an organism can grow; a fast growing organism contains, and indeed requires, a high quota, while if the quota is low then growth is limited. At the extreme, the quota (Q) varies between a minimum value (Q_{\min}), which is the so-called subsistence quota at which growth is not possible, and a maximum (Q_{\max}) at which level the growth rate may attain its maximum value.

Cell-quota vs C-quota

Droop’s quota model used a cell basis. Many still refer to “cell-quota” even if they do not actually use the cell as the core unit for the model structure, or indeed use the Droop equation itself. Michael Droop used the cell as the core unit for the pragmatic reason that he counted cells; he did not measure C-biomass.

There is a problem in using the concept of a “cell-quota”, however. Very simply, phytoplankton cell size changes over the course of growth (doubling and halving over the cell cycle), and the average size also changes in response to temperature (size increase as temperature falls), light (size decreases as light becomes limiting), N-nutrient (size decreases as N becomes limiting) and P-nutrient (size increases as P becomes limiting). Biochemistry relates to chemical concentrations within the cell, and using a C-quota thus provides some form of linkage to that reality.

Relating quota to growth rate

Although, in conversation to the author, Michael Droop was adamant that he saw only an empirical relationship between the (cell) quota and the potential for growth, it is quite easy to make the argument for some mechanistic relationship. Considering N, an organism uses this element for DNA, RNA and proteins. These may be categorised into structural components (DNA and structural proteins) and rate-controlling components (RNA, enzymes etc.). The minimum quota (Q_{\min}), at which point growth rate is zero, thus defines an organism containing only the minimum configuration of structural components plus house-keeping functional components. As the concentration of functional components increases thus the capacity for growth increases towards a maximum. For N that relationship is essentially linear, which is perhaps to be expected. Furthermore, because N cannot be deposited to any significant extent in a form that is not contributing to function (in contrast, P can be deposited within many microbes in large excess, as polyphosphate), the maximum quota (Q_{\max} , in our model as NC_{\max}) aligns pretty well with the maximum growth rate potential.

It must be stressed that the maximum quota does not assure a maximum growth rate; growth may be limited by another factor such as light for photosynthesis, or availability of another nutrient. As

an additional complication, the quota for the non-limiting nutrient may increase under such situations. Thus N:C increases beyond NC_{max} under light-limited growth, eventually attaining an absolute maximum value (which we could term NC_{abs}) limited by cellular biochemistry. Somehow we need to control all of these interactions. But we are getting ahead of ourselves – here we consider the simplest situation of just N-limitation (rather like we did for our very first model, in Chapter 4). The complexities of reality can be reviewed in Flynn (2001, 2008a, 2008b).

For the N:C-quota we thus have a functional relationship that looks like that in Fig. 15.1, giving a linear relationship for growth when it is limited by N:C between the minimum (NC_{min}) and maximum (NC_{max}) quotas of $NC=0.05$ and $NC=0.15$, respectively.

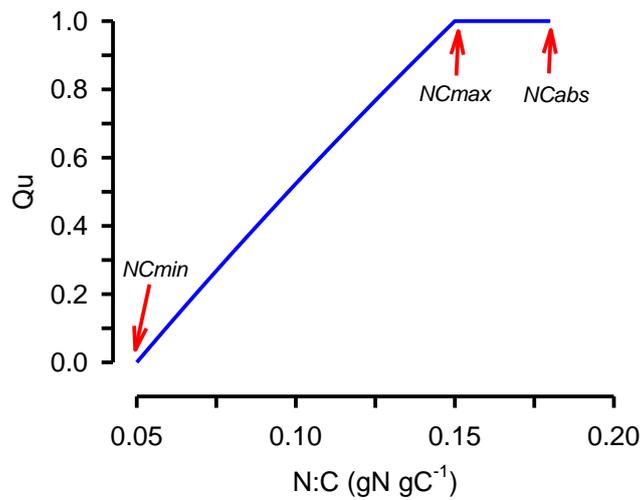


Fig. 15.1 Relationship between the N:C quota quotient and normalised growth rate (Q_u). Here, the minimum quota (NC_{min}) is 0.05, and the maximum quota (NC_{max}) affecting growth rate is 0.15. The absolute maximum quota (NC_{abs}) is shown here at 0.18.

There are various forms of the quota-growth relationship. The original (Droop) version contained a hypothetical maximum growth rate value, and a curve form that was fixed. The equation is not flexible and introduces a parameter (the hypothetical growth rate maxima) that is difficult to relate to any real parameter. The form that we shall use (its derivation is explained in Flynn 2008a, 2008b) provides a curve that yields a growth rate that is normalised (i.e., it reports a nutrient status ranging between 0 and 1), thus simplifying its use in any function that requires reference to an index of nutrient status, and linkage with any required maximum growth rate value. It also contains a curve-shaping constant that can be readily altered to conform to expectations for a particular combination of nutrient and organism (Flynn 2008b).

The formal version of this equation is –

$$Q_u = \frac{(1+KQ) \cdot (Q - Q_{min})}{(Q - Q_{min}) + KQ \cdot (Q_{max} - Q_{min})} \quad \text{Eq.15.1}$$

Here, Q is the current quota value that ranges between Q_{min} and Q_{max} , KQ is a curve shaping constant, and Q_u is the resultant quotient describing the nutrient-status for nutrient quota Q . For a linear relationship, KQ needs to be larger than 5; when considering the quota in terms of N:C a value of 10 is suitable here, while if we were considering P:C not only would the values of Q_{min} and

Q_{max} be very different but also KQ would be much lower (ca. 0.5) giving the response curve a distinctly curvi-linear form (Flynn 2008a, 2008b).

If you look at this equation carefully you will see that the value of $(Q-Q_{min})$ takes the role of a substrate in what is a modified rectangular hyperbolic equation. The value of $(Q_{max}-Q_{min})$ scales the value of this “substrate” across the potential range of Q . The involvement of $(1+KQ)$ in the numerator ensures that the output is a quotient irrespective of the value of KQ .

What, physiologically for the phytoplankton cell, does a change in N:C reflect?

It is perhaps easier to answer this question if we invert the ratio, to C:N; thus $NC_{min} = 1/CN_{max}$, and $NC_{max} = 1/CN_{min}$. When photosynthesis continues in the absence of concurrent N uptake and assimilation, the cell accumulates excess photosynthate in the form of (depending on the organisms taxonomy) starches and/or lipids.

The difference between C:N and C:N_{min} is largely explained by the amount of accumulated C-reserve. The value of CN_{min} (i.e., $1/N:C_{max}$) reflects the stoichiometry of the core cellular structure and machinery in terms of DNA, RNA, protein structural lipids, and the like. The amount of this reserve (C_{res} , as g reserve-C per g biomass C) is given by:

$$C_{res} = \frac{CN - CN_{min}}{CN} \quad \text{Eq.15.2}$$

The numerator gives the value of the amount of C-reserve as the difference between the current C:N (CN) and the value of C:N in a cell which has no reserve (CN_{min}). The denominator then ratios that reserve to the total C, with the units for N cancelling out (leaving units for C_{res} of gC gC⁻¹).

The value of C_{res} is of importance for those attempting to optimise algal growth for fatty acid or biofuels production. This is an interesting exploitation route for stoichiometric models because the maximum content of C_{res} is given in cells that have $CN=CN_{max}$ ($=1/NC_{min}$); and we have established that a cell with $NC=NC_{min}$ has a grow rate of zero. Clearly a maximum production of C_{res} requires some level of growth that falls at an intermediate level between maximum growth when C_{res} is minimal (≈ 0), and zero growth when C_{res} is maximum. Such applied (commercial) applications of quota-based models are considered in Kenny & Flynn (2016) and Flynn et al. (2017).

15.4 Building the Model

The model contains 3 state variables in total. The external N-source (Am) is taken up and leads to an elevation in cellular N (N_{Phy}); that uptake of N is a function of the concentration of Am and also of the removal rate per unit of C-biomass (C_{Phy}). The growth of C_{Phy} is itself a function of phytoplankton N:C (NC_{Phy}); it is not a direct function of Am .

The whole model is visualised in Fig. 15.2, with a full description of parameters in Table 15.1.

Changes in A_m

The initial value of A_m is set by the value of constant $init_A_m$. There is provision for a chemostat dilution defined by $in_out_A_m$. The dilution rate (dil) is defined in this model as a value relative to u_{max_Phy} . In consequence, if $relDil$ is set at 0.5, then the residual value of A_m at steady state reports the half saturation value for growth rate (k_g). Note that in this model the value of k_g is an emergent property, while in the model we built in Chapter 4 it was an input variable (i.e., a constant).

A_m is removed to support growth of N_Phy via Nup .

Changes in N_Phy

The initial value of N_Phy needs to be set such that the ratio of $N_Phy : C_Phy$ (NC_Phy) is within the bounds of $NCmin_Phy$ to $NCmax_Phy$. Here the initial value of N_Phy is set by $C_Phy * NCmin_Phy$, so the cells are described as starting off under extreme N-stress.

The transfer of N from A_m to N_Phy is controlled in the same way that we have used previously (e.g., Chapter 4), making use of a rectangular hyperbola with reference to a half saturation constant. We will term this constant $ktAm_Phy$, representing the control of nutrient transport; as mentioned above this is not the half saturation constant for growth.

The maximum rate of A_m transport needs to be able to support the maximum C-specific rate of phytoplankton growth (as set by u_{max_Phy}) and this rate, as considered above, must align with the needs of the organism when the value of cellular N:C is at its maximum (i.e., when $NC_Phy = NCmax_Phy$). The maximum rate of C-specific N-transport into the cell ($TNmax_Phy$; $gN\ gC^{-1}\ d^{-1}$) at that time must thus be given by $u_{max_Phy} * NCmax_Phy$.

The actual rate of C-specific N-transport is then given by NCt_Phy ($gN\ gC^{-1}\ d^{-1}$), via the rectangular hyperbolic term relating to substrate availability. Accounting for the total current algal C-biomass (C_Phy ; $\mu g\ C\ L^{-1}$), the population uptake of N (Nup ; $\mu g\ N\ L^{-1}\ d^{-1}$) is defined as $NCt_Phy * C_Phy$.

Washout by dilution of N_Phy is described by $outN_Phy$.

Note that it is critically important that all such loss terms applied to N_Phy must be applied to C_Phy , and vice versa.

Quota control on growth

The current nutrient status of the cells in the culture is defined by reference to the N:C quota, NC_Phy . As a C-quota based quotient, the nutrient status (NCu_Phy) is described through reference to the minimum and maximum quotas ($NCmin_Phy$ and $NCmax_Phy$, respectively), and the quota-curve constant KNQ_Phy . The value of NCu_Phy thus defines the optimum N-status as 1, with a value of 0 being the lowest N-status.

Changes in C_Phy

The C-specific growth rate of the phytoplankton (u_Phy) is now a product of NCu_Phy and the maximum growth rate, u_{max_Phy} . The population growth ($groC_Phy$) is given as $u_Phy * C_Phy$. There is also a washout rate by dilution, described by $outC_Phy$.

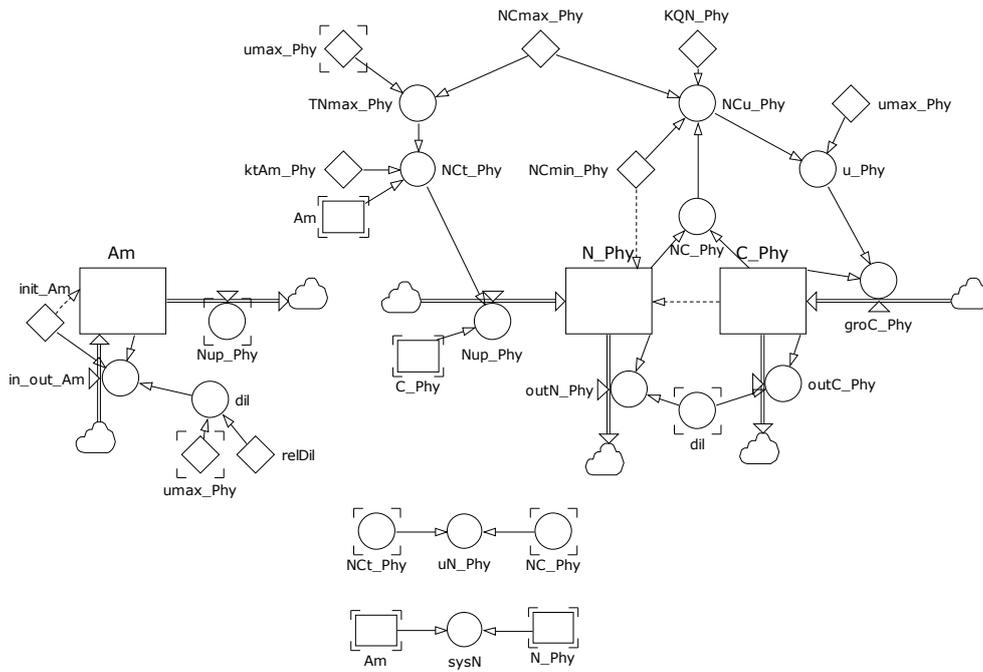


Fig. 15.2 Simple NC quota phytoplankton model. See also Table 15.1.

Other parameters

The other parameters that are of use (Table 15.1) are the system-N (*sysN*), and also the phytoplankton N-specific growth rate (*uN_Phy*).

It is worth noting that no attempt is made here to balance system C; to do so would require reference to dissolved inorganic C as the C-source, and assume that the system was sealed gas-tight.

15.5 Parameterising the Model

In many ways, parameterising this model is an extension of methods described in Chapter 4. The added complication is of course that we now need measurements of both C and N biomass. If you wished to establish the system C then you would need to operate a sealed culture vessel, and take measurements of dissolved inorganic carbon from the growth medium.

| Name | Type | Definition | Unit | Documentation |
|------------------|------|---|--------------------------------------|---|
| <i>Am</i> | SV | $init_Am$ $+ dil*(init_Am-Am)$ | $\mu\text{g N L}^{-1}$ | Ammonium-N |
| <i>C_Phy</i> | SV | 12 $+ groC_Phy$ $- outC_Phy$ | $\mu\text{g C L}^{-1}$ | Phytoplankton-C |
| <i>N_Phy</i> | SV | $C_Phy*NCmin_Phy$ $+ Nup_Phy$ $- outN_Phy$ | $\mu\text{g N L}^{-1}$ | Phytoplankton -N |
| <i>init_Am</i> | Con | 14*10 | $\mu\text{g N L}^{-1}$ | Input ammonium-N |
| <i>KQN_Phy</i> | Con | 10 | dl | KQ for N-quota |
| <i>ktAm_Phy</i> | Con | 14 | $\mu\text{g N L}^{-1}$ | Half saturation constant for ammonium transport |
| <i>NCmax_Phy</i> | Con | 0.15 | gN gC^{-1} | Maximum <i>NC_Phy</i> |
| <i>NCmin_Phy</i> | Con | 0.05 | gN gC^{-1} | Minimum <i>NC_Phy</i> |
| <i>relDil</i> | Con | 0 | dl | Dilution rate relative to <i>umax_Phy</i> |
| <i>umax_Phy</i> | Con | 0.693 | $\text{gC gC}^{-1} \text{d}^{-1}$ | Maximum C-specific growth rate |
| <i>dil</i> | Aux | $umax_Phy*relDil$ | d^{-1} | dilution rate |
| <i>groC_Phy</i> | Aux | C_Phy*u_Phy | $\mu\text{g C L}^{-1} \text{d}^{-1}$ | Growth rate in phytoplankton-C |
| <i>in_out_Am</i> | Aux | $dil*(init_Am-Am)$ | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | Nutrient exchange |
| <i>NC_Phy</i> | Aux | N_Phy/C_Phy | gN gC^{-1} | Phytoplankton N:C quota |
| <i>NCT_Phy</i> | | $TNmax_Phy*Aml(Am+ktAm_Phy)$ | $\text{gN gC}^{-1} \text{d}^{-1}$ | Phytoplankton C-specific N transport rate |
| <i>NCu_Phy</i> | Aux | $(1+KQN_Phy)*(NC_Phy-NCmin_Phy)/((NC_Phy-NCmin_Phy)+KQN_Phy*(NCmax_Phy-NCmin_Phy))$ | dl | Quotient for N-status |
| <i>Nup_Phy</i> | Aux | $C_Phy*NCT_Phy$ | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | Phytoplankton population uptake of ammonium-N |
| <i>outC_Phy</i> | Aux | $C_Phy*dil$ | $\mu\text{g C L}^{-1} \text{d}^{-1}$ | Washout of <i>C_Phy</i> |
| <i>outN_Phy</i> | Aux | $N_Phy*dil$ | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | Washout of <i>N_Phy</i> |
| <i>sysN</i> | Aux | $Am+N_Phy$ | $\mu\text{g N L}^{-1}$ | System N |
| <i>TNmax_Phy</i> | Aux | $umax_Phy*NCmax_Phy$ | $\text{g N gC}^{-1} \text{d}^{-1}$ | Maximum C-specific N-transport rate |
| <i>u_Phy</i> | Aux | $umax_Phy*NCu_Phy$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | C-specific growth rate controlled by N:C quota |
| <i>uN_phy</i> | Aux | NCT_Phy/NC_Phy | $\text{gN gN}^{-1} \text{d}^{-1}$ | N-specific growth rate |

Table 15.1 Parameter descriptions for a simple NC quota model. See also Fig. 15.2. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

15.6 Operating the Model

An example output is given in Fig. 15.3. There is no dilution applied in this instance, so growth proceeds according to batch culture kinetics.

Note that N-specific growth (u_{N_Phy}) is very high to start; as the N-starved cells undergo up-shock they fill with ammonium-N and the value of NCu_Phy rises to near its maximum value of 1. N-specific and C-specific growth rates are at this stage now matched (i.e., the organism physiology is in near-steady-state) and this situation continues for a few days until Am becomes limiting. The external nutrient (Am) falls away to approach zero by ca. day 7, as does the value of N-specific growth. C-specific growth (u_Phy), however, continues at a slowly declining rate over the next week in the absence of concurrent new N-assimilation.

The plots of C-specific growth and N-specific growth thus show contrasting forms. Also, the population growth curves plotted with respect to phytoplankton N-biomass (N_Phy) differs significantly from that for C-biomass (C_Phy). In real organisms, continued growth in the absence of concurrent new N assimilation would be achieved through a redirection of previously assimilated N to essential biochemical processes. The model output thus demonstrates the dangers of describing “specific growth rate” values without reference to the full units explaining the origin of the rate derivation (see Section 4.5).

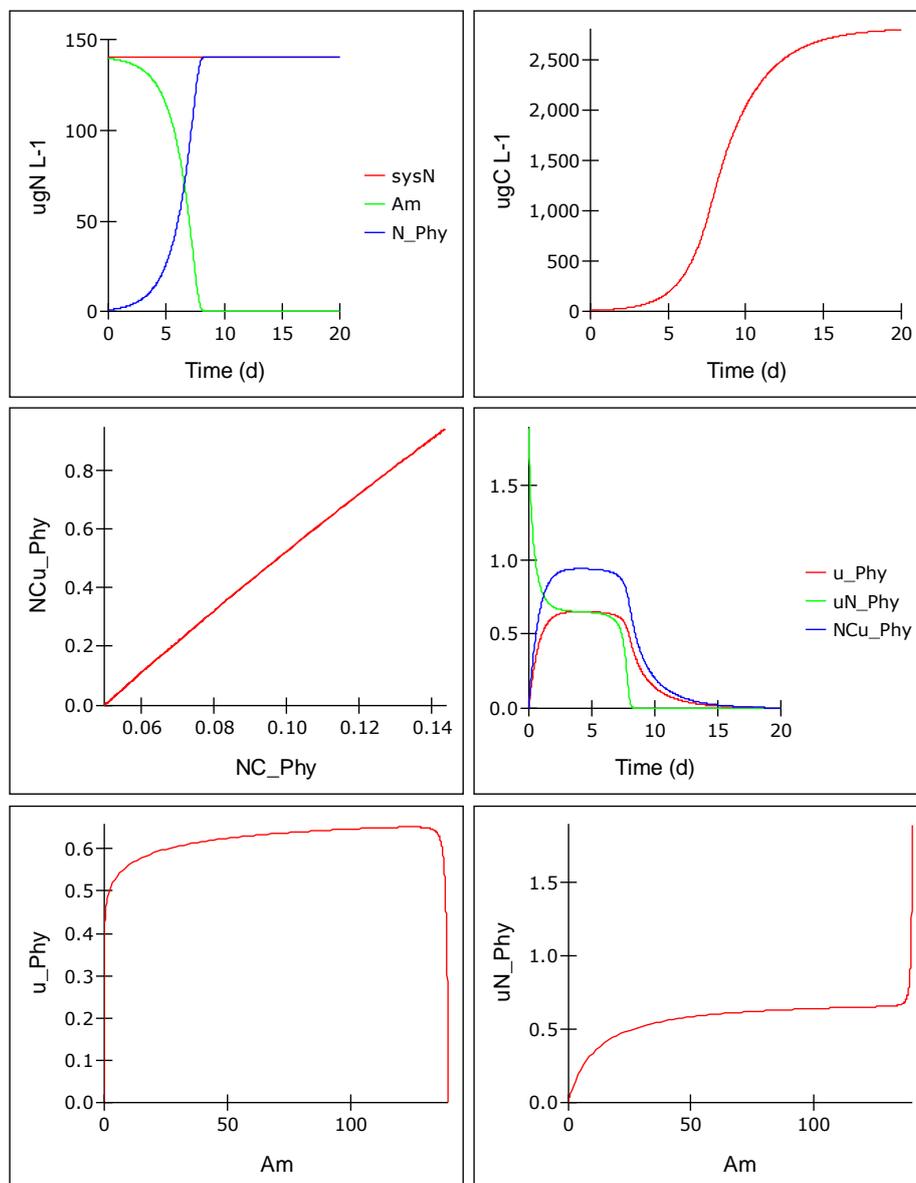


Fig. 15.3 Example model output, operating in batch culture mode (i.e., $relDil = 0$).

15.7 Things to Explore

- i) Modify the model to include a definition of the C-reserve (C_{res} ; Eq.15.2). Develop a description of the production of C_{res} , and then explore the relationship between dilution rates and C_{res} production that could inform the commercial exploitation of microalgae for biofuels.
- ii) How does altering NC_{min_Phy} (between ca. 0.025 and 0.14 gN gC⁻¹) and the value of u_{max_Phy} (between ca. 0.35 and 1.2 d⁻¹; see Flynn & Raven (2017) for a discussion about how high this value can become) affect the dynamics of growth, and the results of your deliberations for (i) above? If you set NC_{min} very close to NC_{max} , you essentially negate the implications of variable stoichiometry and quota control of growth. The model will then behave in a similar fashion to that you built in Chapter 4.
- iii) Build in a link between the concentration of dissolved inorganic C (DIC) and C-assimilation as defined in the current structure at $groC_Phy$. DIC in seawater is present at ca. 2mM, while the half saturation constant for its use is ca. 100 μ M (Clark & Flynn 2000). Assume a Monod-style relationship controlling growth by DIC concentration. What do the kinetics of growth look like now, and how much N (as Am) can you add before growth becomes co-limited by N and DIC? What implications does this have for growing cultures in static (non-aerated) flasks?
- iv) If you set $relDil = 0.5$, the resultant value of Am at steady-state equates to the value of the half saturation concentration for growth (i.e., k_g). Repeat exploration (ii), above, and see how the value of k_g changes. What does this tell you about the configuration of phytoplankton to optimise competitive advantage when limited by a single N-source?
- v) Test your hypothesis from (iv) by building another phytoplankton model that consumes the same state variable of Am . Configure your two competing phytoplankton differently with respect to their input variables.
- vi) Build in self shading (see Chapter 8). Replacing Nu in Table 8.1 with NCu_Phy from Table 15.1 will provide the linkage from nutrient stress to controlling the maximum photosynthetic rate. The flip side is to control nutrient uptake in consequence of light-limitation. A way of doing this that accords with algal physiology is to provide a feedback from N:C to halt N transport. Thus as N:C increases from NC_{max} towards NC_{abs} (Fig. 15.1) so TN_{max_Phy} is decreased to zero. As a crude approach you could just make $TN_{max_Phy} = 0$ if $NC_Phy > NC_{max_Phy}$.

15.8 Caveats

- The main caveat is the absence of light limitation; you could build that in by extending the approach used in Chapter 8 (see Section 15.7 vi). More appropriately, the model should ideally also simulate photoacclimation, through changes in Chl:C influenced both by the irradiance received by the cells, and by their nutrient status (see Flynn 2001, Flynn et al. 2001).
- There is an assumption made with this model that no other nutrients are limiting. This structure has no capacity for combining, for example, N and P co-limitation. Such interactions, and the way that quota-style approaches are used to handle them, provide a wide range of opportunities for exploration through simulations. Examples of such models

and of implications of their formulation on simulations are in Flynn (2001, 2003, 2005 & 2008a).

- Other caveats are similar to those in Chapters 4 & 8.

15.9 Where Next

Here we linked a more detailed description of internal physiology to the same simple description of nutrient uptake that we used earlier. There are various papers in the literature that you could explore to guide you in replacing the transport term used here with one that takes account of three important features that affect how real phytoplankton behave, namely diffusion limitation of the availability of nutrients at the site of transport into the cells, the development of transporters to enhance acquisition, and the effect of cell size and motility on the processes.

In the next chapter we consider the implications of variable stoichiometry on predator-prey dynamics.

16. Variable Stoichiometric Predator-Prey Interactions

Terms and concepts introduced in this chapter- palatability, quantity of food, quantity of food, voiding, regeneration, gross growth efficiency, harmful algal bloom (HAB), ecosystem disruptive algal bloom (EDAB), trait-trade-offs.

16.1 Ecological Context

As introduced in the previous chapter, differential stoichiometry between members of a trophic web has the ready potential to significantly affect the dynamics of ecology. Having built a description of phytoplankton growth describing variable stoichiometry (Chapter 15), and hence variable nutritional value for a consumer, here we build a consumer model to feed upon it.

Even though we make the assumption that the elemental stoichiometry of the consumer is fixed (here, as C:N), as you will see there is plenty of scope for considering interactions linking both the quantity and quality of the phytoplankton prey to consumer feeding and growth. Throughout the following the text couple *predator-prey* will be used, though in most instances *consumer-food* would apply equally.

The factors that we will consider include the following:

- i) The transfer of elements between prey and predator depends in large measure upon the difference in their chemical constitution. An excess of N in the feed must be discarded (there is no scope to store or assimilate it in a heterotroph; there would be if the predator was a mixotroph as it would have an additional set of biochemical pathways to reintroduce inorganics). Even where N is limiting, inevitably some loss of N from the food must occur, associated with inefficiencies in digestion, and in association with SDA (Chapter 5). If there is an excess of C then this must also be discarded, though some portion of it may be consumed in support of respiration; if this was not undertaken then even more N would have to be discarded.
- ii) If the prey is of poor nutritional value then its digestion may be less efficient. The consumer could potentially increase its feeding rate to counter such a decrease in assimilation efficiency (AE) which would maintain the predators' growth rate but decrease the conversion efficiency of prey biomass into predator biomass.
- iii) If there is an abundance of prey (and in general, an abundance of food) then the predators may likely become less efficient in handling it. This leads to density dependent inefficiency (Flynn 2009) and a decrease in AE. This in turn again results in a loss in trophic transfer up the food web for a given rate of consumption of lower trophic levels (Cf. (ii)). It should be noted that the value of AE *per se* is not of consequence to the predator; all that is of consequence is the rapid growth of the individual predator in competition with other predators.
- iv) Nutrient-deprived phototrophs may produce secondary metabolites which can be noxious or even toxic. Such chemicals may result in rejection by the predator of the organism as prey. The relationship between nutrient-status and palatability may be strongly non-linear, with only a slight deterioration in prey stoichiometry leading to complete rejection by the predator (Mitra & Flynn 2006a).

- v) The form in which C and N is lost from the predator is important for the operation of the whole food web. We need to account for the difference between voided organics, and inorganics.

As can be seen, even our “simple” zooplankton model will actually be quite complex, giving a lot of scope for *in silico* experimentation.

The new zooplankton model is shown in Fig. 16.1, and variables tabulated in Tables 16.1, 2 & 3. What follows is an explanation for the structure. The model is developed from that of Mitra (2006).

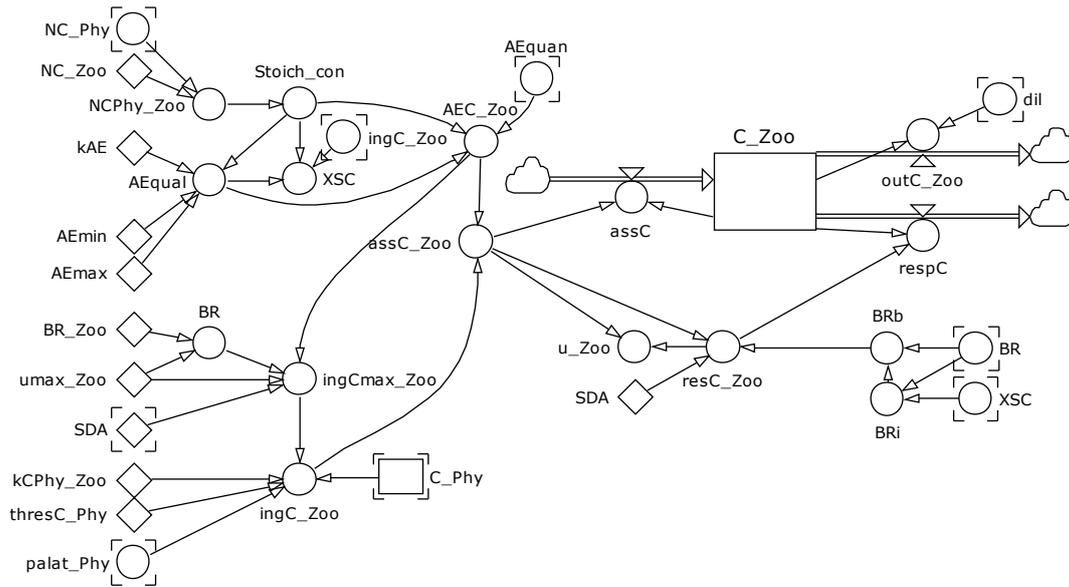


Fig. 16.1 Schematic of the zooplankton model. See Tables 16.1, 16.2. Note that this sub-model needs to be added to that developed in Chapter 15.

| Variable | Type | Value | Unit | Description |
|------------|------|--------------------------------------|---------------------|---|
| C_Phy | SV | {see Table 15.1} | µgC L ⁻¹ | Phytoplankton C-biomass |
| C_Zoo | SV | 1 + assC - respC - outC_Zoo | µgC L ⁻¹ | Zooplankton C-biomass |
| AEmax | Con | 0.6 | dl | Maximum AE for N |
| AEmin | Con | 0.2 | dl | Minimum AE for N |
| BR_Zoo | Con | 0.1 | dl | Basal respiration as a proportion of umax_Zoo |
| kAE | Con | 1.00E+03 | dl | Constant for control of AE in response to prey quality |
| kCPhy_Zoo | Con | 140 | µgC L ⁻¹ | Half saturation of zooplankton predation on phytoplankton |
| kGTT | Con | 100 | µgC L ⁻¹ | Curve control for density dependant inefficiency |
| minAE_mult | Con | 1 | dl | Minimum AEC scalar for density dependant inefficiency |
| NC_Zoo | Con | 0.2 | gN gC ⁻¹ | N:C of zooplankton |
| SDA | Con | 0.3 | dl | Specific Dynamic Action |
| thresC_Phy | Con | 0.014 | µgC L ⁻¹ | Threshold for predation upon phytoplankton |
| tox_Phy | Con | 0.6 | dl | Toxicity scalar |
| umax_Zoo | Con | 0.693 | d ⁻¹ | Zooplankton maximum growth rate |

Table 16.1 Constants and state variables for the zooplankton sub-model. dl dimensionless. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

| Variable | Type | Value | Unit | Description |
|--------------------|------|--|-------------------------------------|---|
| <i>AEC_Zoo</i> | Aux | $Stoich_con * AEqual * AEquan$ | dl | Operational AE for C |
| <i>AEqual</i> | Aux | $\frac{AEmin + (AEmax - AEmin) * Stoich_con / (Stoich_con + kAE) * (1 + kAE)}{(1 - minAE_mult) * (1 - C_Phy / (C_Phy + kGTT)) + minAE_mult}$ | dl | Efficiency parameter for assimilation |
| <i>AEquan</i> | Aux | $\frac{(1 - minAE_mult) * (1 - C_Phy / (C_Phy + kGTT)) + minAE_mult}{C_Zoo * assC_Zoo}$ | dl | AEC scalar for density dependant inefficiency |
| <i>assC</i> | Aux | $C_Zoo * assC_Zoo$ | $\mu\text{gC L}^{-1}$ | Assimilation of C into zooplankton population biomass |
| <i>assC_Zoo</i> | Aux | $AEC_Zoo * ingC_Zoo$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Assimilation rate into zooplankton |
| <i>BR</i> | Aux | $umax_Zoo * BR_Zoo$ | d^{-1} | Zooplankton basal respiration rate |
| <i>BRb</i> | Aux | $BR - BRi$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Balance of basal respiration that cannot be met from dietary excess C |
| <i>BRi</i> | Aux | $IF(BR \leq XSC, BR, XSC)$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Basal respiration that is met by respiration of excess C in diet |
| <i>ingC_Zoo</i> | Aux | $IF(C_Phy > thresC_Phy, palat_Phy * ingCmax_Zoo * (C_Phy - thresC_Phy) / (C_Phy - thresC_Phy + kCPhy_Zoo), 0)$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Ingestion rate of prey into zooplankton |
| <i>ingCmax_Zoo</i> | Aux | $(umax_Zoo * (1 + SDA) + BR) / AEC_Zoo$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Maximum ingestion rate by zooplankton |
| <i>NC_Phy</i> | Aux | {see Table 15.1} | gN gC^{-1} | Phytoplankton N:C |
| <i>NCPhy_Zoo</i> | Aux | NC_Phy / NC_Zoo | dl | Ratio of NC in prey compared to predator |
| <i>outC_Zoo</i> | Aux | $C_Zoo * dil$ | $\mu\text{gC L}^{-1} \text{d}^{-1}$ | Washout of zooplankton biomass |
| <i>palat_Phy</i> | Aux | $(NCu_Phy + 1e-6)^{tox_Phy}$ | dl | Palatability index (0 not palatable) |
| <i>resC_Zoo</i> | Aux | $BRb + assC_Zoo * SDA$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Zooplankton respiration rate |
| <i>respC</i> | Aux | $C_Zoo * resC_Zoo$ | $\mu\text{gC L}^{-1} \text{d}^{-1}$ | Zooplankton population respiration |
| <i>Stoich_con</i> | Aux | $MIN(NCPhy_Zoo, 1)$ | dl | Selection of release of N related to difference in food to consumer N:C |
| <i>u_Zoo</i> | Aux | $assC_Zoo - resC_Zoo$ | d^{-1} | Zooplankton growth rate |
| <i>XSC</i> | Aux | $IF(Stoich_con < 1, AEqual * ingC_Zoo * (1 - Stoich_con), 0)$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | C available for support of respiration |

Table 16.2 Auxiliaries for the zooplankton sub-model. dl dimensionless.

16.2 Handling Differential Stoichiometry between Prey and Predator

We start by considering the difference between prey NC (*NC_Phy*) and its predator (*NC_Zoo*) by taking the ratio of these (to give *NCPhy_Zoo*). This tells us in relative terms how lacking the food is, in terms of N, for the consumer. The prey could, of course, have a higher N:C than the predator; unless the predator is a mixotroph then even under the impossible scenario of a 100% transference this situation must result in a loss of N. We thus need to limit the value of *NCPhy_Zoo* to 1 to give a control index for stoichiometry (*Stoich_con*).

We now come to the first of the food-quality linkages. The value of *Stoich_con* gives an index of food quality, and this can be used to modify the operational value of assimilation efficiency for the limiting nutrient. This value, *AEqual*, ranges between minimum and maximum values (*AEmin* to

AE_{max}), with the shape of this relationship controlled by the value of a constant, kAE . Different response forms can be readily considered; see Fig. 16.2. Note that AE_{min} in this equation does not align with the value of AE_{equal} given at the lowest NC_{Phy} , but at a hypothetical value of $NC_{Phy}=0$.

The default value of AE for the non-limiting element, which is C, is given as the product of $Stoich_{con} * AE_{equal}$ ($=AEC_{Zoo}$). Even if there is no quality interaction with AE (as per Fig. 16.2), the AE for C cannot be higher than that for the element in shorter supply, N.

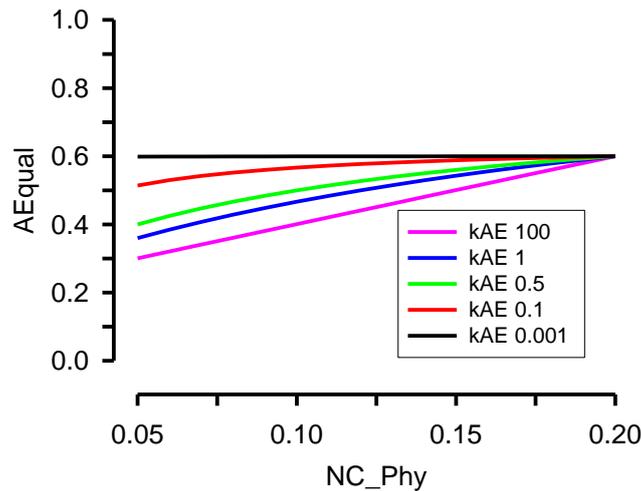


Fig. 16.2 Food quality control on AE for the limiting nutrient. Varying the value of kAE (as indicated) alters the relationship between prey N:C (NC_{Phy}) and the value of AE_{equal} .

16.3 Prey Excess – Superfluous Feeding and Density Dependant Inefficiency

All consumers handle and/or process food less efficiently when that food is present in abundance. This is in part a behavioural activity at feeding itself, but it is also partly a function of digestion after feeding. Organisms with a gut, and indeed also unicellular grazers, process food for a certain period of time before discarding the remnants; the food is *de facto* on a conveyer belt, the speed of which is affected by the amount of material upon it and the availability of new food being added to it. If there is plenty of food available then the time taken to pass through the digestion process, which for an animal with a gut is termed the gut transit time (GTT), is decreased. There is no advantage in expending resources digesting the last part of a meal when the next one is available for initial rapid and more efficient digestion. If we built a food-processing model with an explicit representation of a gut (e.g., Mitra & Flynn 2007) we could explicitly describe GTT, but as the consequence of decreasing GTT is to decrease AE we will involve just that end result in our model here.

The basis of this interaction in reality is satiation; we could relate satiation to the value of $ingC_{Zoo}/ingC_{max_Zoo}$. However, we cannot simply involve the value of $ingC_{Zoo}$ to alter the value of AE as this generates a circular argument (a mathematical short-circuit, if you like). We could take the value of $ingC_{Zoo}$ at the previous time-step and use that to inform a new value of AE . Alternatively, to describe it in a simple fashion we need to make the assumption that if prey

are available then they will be eaten, and thus relate AE to the abundance of prey; this is the route we will take here.

The form of the response curve is shown in Fig. 16.3. The equation (Eq.16.1) is based around an inverted rectangular hyperbola operating over a limited (closed) output range, but with an open input (0 to whatever the prey abundance is) with reference to what amounts to a half saturation value, $kGTT$. The value of AE_{quan} is used to modulate the value of AE .

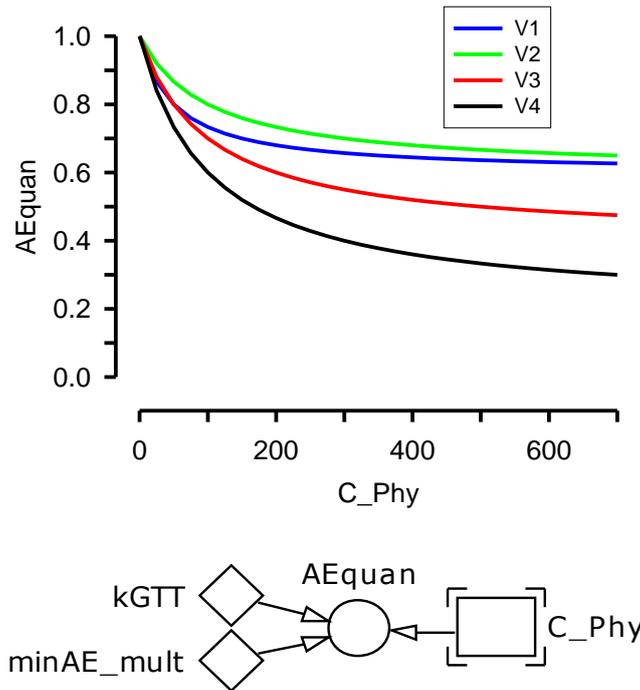


Fig. 16.3 Response curve and sub-model relating prey abundance (C_{Phy} , and thus through inference satiation of the digestive process in the predator) to a scalar, AE_{quan} , to modify the value of AE . The values of $kGTT$ and $minAE_mult$ for each of the curves are respectively: v1 – 50, 0.6; v2 – 100, 0.6; v3 – 100, 0.4; v4 – 100, 0.2. See also Table 16.2.

$$AE_{quan} = (1 - minAE_mult) * (1 - C_{Phy} / (C_{Phy} + kGTT)) + minAE_mult \tag{Eq.16.1}$$

To turn the function off, simply set $minAE_mult = 1$.

The value of AE_{quan} is used to further modify the value of AEC_{Zoo} , which is now given by $Stoich_con * AEqual * AEquan$.

16.4 Palatability and Prey Ingestion

Now we have a value of AEC_{Zoo} we can establish the maximum feeding rate ($ingCmax_{Zoo}$) required to support the maximum growth rate ($umax_{Zoo}$), set against the inefficiencies and respiratory losses. This approach is similar to that we used in Chapter 5; **but see Section 16.13**. The actual ingestion rate is a function of prey abundance, here described using a rectangular hyperbolic term, with reference to half saturation constant $kCPhy_{Zoo}$. Note that while the

analogous constant in the model in Chapter 5 is N-based, this one is C-based; in consequence the numeric value will differ, reflecting the value of NC_Phy . The same applies to the threshold below which predation does not occur (introduced to prevent extinction of the prey); $thresC_Phy$ has units of $\mu\text{gC L}^{-1}$. It should thus be clear that the food value of a given phytoplankton cell will decrease as its N:C decreases. Via $AEqual$, that deterioration may be faster still upon digestion. But the deterioration in value as a food source may be far greater again if the decline in phytoplankton N:C is associated with chemical changes that decrease palatability. And it is to that we turn next.

If the palatability of food decreases, it does not matter how hungry you are, you do not eat so much, or at the extreme you reject the food completely. So, in the model we now introduce a palatability term that decreases the effective value of $ingCmax_Zoo$ at the point of calculating $ingC_Zoo$. We relate palatability to the N-status of the phytoplankton via the value of the quotient NCu_Phy (Chapter 15, Table 15.1), and to the input variable, tox_Phy (Fig. 16.4) to describe a decrease in palatability as the level of N-stress increases (Fig. 16.4; Eq.16.2).

$$palat_Phy = (NCu_Phy + 1e-6)^{tox_Phy} \tag{Eq.16.2}$$

The presence of "1e-6" in Eq.16.2 is to prevent 0^{tox_Phy} , which will generate a mathematical error, should NCu_Phy decline to 0.

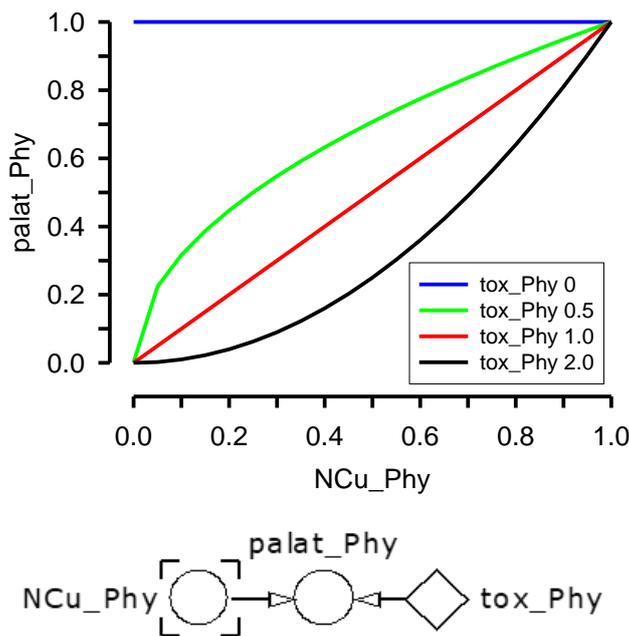


Fig. 16.4 Nutrient stress (NCu_Phy) control over phytoplankton palatability ($palat_Phy$). The different response curves are given using the indicated values of tox_Phy .

The variable $palat_Phy$ is a quotient for palatability which is then applied in the calculation of $ingC_Zoo$. As an alternative, you could build the model to apply the value of $palat_Phy$ in some way to the half saturation constant, making $kCPhy_Zoo$ larger as palatability decreases; this would not affect the maximum ingestion rate, but would introduce a change in preference. You could also build the response curve so that it does not decrease grazing to zero.

Remember, always build your response curves in a spreadsheet to test what the function looks like using different input variables before implementing it in your model.

16.5 Assimilation, Respiration and Growth

We now have a C-specific ingestion rate, with units of g prey-C per g predator-C per day. From this we obtain the C-specific assimilation rate ($assC_{Zoo}$) and thence the population assimilation rate ($assC$) (Fig. 16.1; Tables 16.1, 16.2). Next we need to derive the respiration rates, and then the growth rate.

As before (Chapter 5) we have a basal respiration rate (BR) which is itself defined as scaled to $umax_{Zoo}$ by BR_{Zoo} . This can be supported by “burning” off some of the zooplankton C-biomass and/or by using any excess C that enters from assimilation of the incoming prey. The entry of excess of C in the diet, which is referenced to the N:C of the predator, is given by XSC :

$$XSC = IF(Stoich_con < 1, AEqual * ingC_{Zoo} * (1 - Stoich_con), 0) \quad Eq.16.3$$

XSC is only available if the value of $NC_{Phy}/NC_{zoo} < 1$; this is tested by $Stoich_con < 1$. Provided that condition is met, however, the function returns the rate of ingestion of C that is not bound to N in the proportion required to match the zooplankton biomass N:C. In this model we do not allow this excess C to accumulate; in a real consumer some level of C-storage (usually as fat) occurs, and supports basal respiration during periods of starvation. Only when this store is exhausted does the consumer have to burn off proteins. To describe such functionality would require a variable stoichiometric description of the zooplankton, with an additional state variable describing fat.

To cover the cost of BR , the first recourse is to consume XSC . The rate of support via XSC is:

$$BRi = IF(BR \leq XSC, BR, XSC) \quad Eq.16.4$$

The value of BR that cannot be covered from the diet (and must thus come from “burning” predator biomass) is given by:

$$BRb = BR - BRi \quad Eq.16.5$$

The total C-specific respiration from the assimilated C, including respiration associated with anabolism via SDA (see Section 5.4) is then given as:

$$resC_{Zoo} = BRb + assC_{Zoo} * SDA \quad Eq.16.6$$

Total production of CO_2 is the sum of BRi and $resC_{Zoo}$.

With the calculation of the population respirational loss of zooplankton C-biomass ($respC$), and the washout of that biomass by chemostat-style dilution ($outC_{Zoo}$) the main zooplankton model is complete (Fig. 16.1). However, we still have to resolve the fate of materials that are voided and respired.

16.6 Voided Organics

Ingested material that is not assimilated is voided. The form of this material is important for the functioning of the ecosystem both with respect to the quantity and also its stoichiometric quality. The sub-model is shown in Fig. 16.5, with variable descriptions in Table 16.3.

It is important to note that “voided organics” comprises both particulate and dissolved materials; the model does not differentiate between them, and in practice the structural identity will vary between different combinations, and nutrient status, of predator and prey (consumer and food). There is also an operational problem in science because the definition of “dissolved organic matter” (DOM) is that the material passes a 0.2µm pore filter; this can exclude forms of DOM that you may think of as dissolved (such as mucus) and include smaller rod-shaped bacteria, microfaecal pellets and so on, that are clearly not dissolved. Most animal faeces is a mix of dissolved and particulate material of different effective size.

The voided C comprises the material that is ingested and not assimilated. The value of this (*void_C_Zoo*) is given by the ingested material (*ingC_Zoo*), minus that stoichiometrically assimilated with N into biomass (*assC_Zoo*), and minus that portion of *XSC* that is not respired (*BRI*).

Voided N is analogous to voided C (*XSassN*), but with one extra detail. While C-metabolites need not be associated with N (e.g., fats and sugars do not contain N), the same is not true of organic-N compounds; organic-N must always include C. And there is a maximum N:C that is possible in organic matter (*NCmax*). If the N:C of the voided matter exceeds this critical value, then a proportion of the N must be released as inorganic-N (as ammonium).

The voided N is thus given by:

$$voidN_Zoo = IF((XSassN/voidC_Zoo > NCmax), voidC_Zoo * NCmax, XSassN) \quad \text{Eq.16.7}$$

Just for information (the value is not used in the workings of the model), the value of N:C in the voided organics is reported by *NC_VO* (Table 16.3); the value is of importance to detritivores as they rely on the stoichiometry of this material for their own growth.

The concentration of *VOC* and *VON* is subjected to the chemostat-style dilution (*out_VOC* and *out_VON*, respectively).

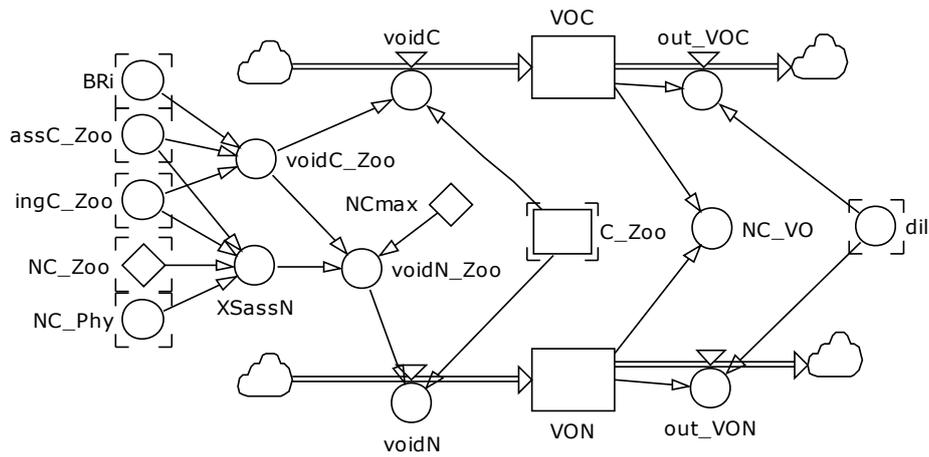


Fig. 16.5 Voided materials sub-model. See also Table 16.3.

| Variable | Type | Value | Unit | Description |
|-----------|------|---|--------------------------------------|--|
| VOC | SV | 0 + voidC - out_VOC | $\mu\text{g C L}^{-1}$ | Faecal material -C |
| VON | SV | 0 + voidN - out_VON | $\mu\text{g N L}^{-1}$ | Faecal material -N |
| C_Zoo | SV | {see Table 16.1} | $\mu\text{g C L}^{-1}$ | Zooplankton C-biomass |
| NC_Zoo | Con | 0.2 | gN gC^{-1} | N:C of zooplankton |
| NCmax | Con | 0.3 | gN gC^{-1} | maximum mass ratio of N:C which could be attained in the organic form |
| DINr | Aux | $(resC_Zoo*NC_Zoo)+(XSassN-voidN_Zoo)$ | $\text{gN gC}^{-1} \text{d}^{-1}$ | Zooplankton ammonium regeneration |
| NC_VO | Aux | VON/VOC | gN gC^{-1} | N:C of voided organics |
| out_VOC | Aux | VOC*dil | $\mu\text{g C L}^{-1} \text{d}^{-1}$ | Washout of voided C |
| out_VON | Aux | VON*dil | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | Washout of voided N |
| recC_Zoo | Aux | {see Table 16.2} | $\text{gC gC}^{-1} \text{d}^{-1}$ | Zooplankton respiration rate |
| reg_Am | Aux | C_Zoo*DINr | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | Zooplankton population regeneration of ammonium |
| voidC | Aux | C_Zoo*voidC_Zoo | $\mu\text{g C L}^{-1} \text{d}^{-1}$ | Population rate of C voiding |
| voidC_Zoo | Aux | ingC_Zoo-assC_Zoo-BRi | $\text{gC gC}^{-1} \text{d}^{-1}$ | Voiding of C by zooplankton |
| voidN | Aux | C_Zoo*voidN_Zoo | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | Population rate of N voiding |
| voidN_Zoo | Aux | IF((XSassN/voidC_Zoo>NCmax), voidC_Zoo*NCmax, XSassN) | $\text{gN gC}^{-1} \text{d}^{-1}$ | Voiding of N by zooplankton |
| XSassN | Aux | ingC_Zoo*NC_Phly-assC_Zoo*NC_Zoo | $\text{gN gC}^{-1} \text{d}^{-1}$ | Amount of N initially in the organic form to be voided to maintain constant predator N:C |

Table 16.3 Voided organic sub-model. dl dimensionless. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

16.7 Ammonium Regeneration

Zooplankton C-specific ammonium regeneration (*DINr*) is associated with respiration involving the “burning” of C-biomass (i.e., $resC_Zoo*NC_Zoo$). It also includes ammonium from that proportion of voided N that cannot be associated with organics (see Section 16.6); this is given by $XSassN-voidN_Zoo$. Total regenerated ammonium (*reg_Am*; Fig. 16.6) generated by the zooplankton

population needs to be introduced as an input to the *Am* state variable which supports growth in the phytoplankton model (see Section 16.9).

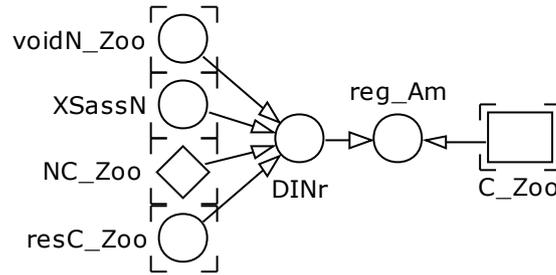


Fig.16.6 Ammonium regeneration sub-model. See also Table 16.3.

16.8 Gross Growth Efficiency

In addition to the assimilation efficiency, which we use in consumer models as an input variable, a variable of interest in defining consumer dynamics is the **gross growth efficiency** (GGE; Fig. 16.7). This describes the total efficiency as the proportion of ingested material that ends up in the consumer biomass. Like assimilation efficiency, there are C and N –specific versions of these. The equations are given in Table 16.4.

As mentioned before, in the context of AE, the meaning of these “efficiencies” should not be used to necessarily infer competitive advantage. A successful strategy for an individual could be to obtain resources as effectively as possible, and only part-digest them thus enhancing gut throughput. When there is plenty of food this could support a high growth rate for the individual, while decreasing the abundance of food for competitors; it is however a strategy that gives low efficiencies in terms of AE and GGE.

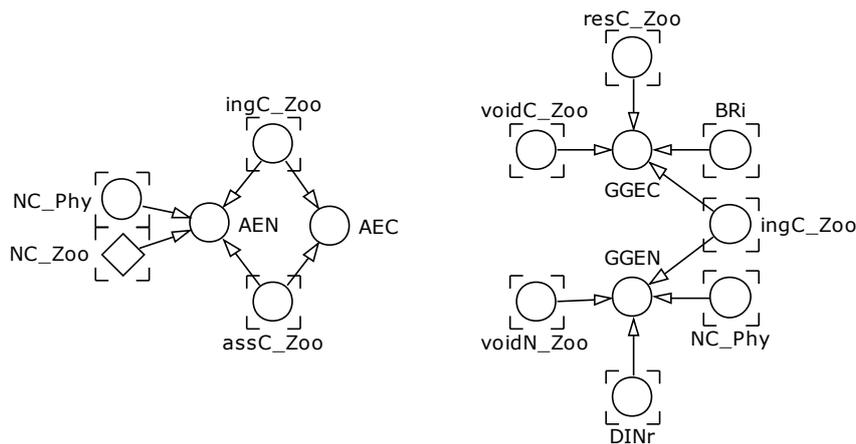


Fig. 16.7 Assimilation and Gross Growth Efficiencies. See Table 16.4.

| Variable | Type | Value | Unit | Description |
|------------------|------|---|-------------------------------------|--|
| <i>NC_Zoo</i> | Con | 0.2 | gN gC ⁻¹ | N:C of zooplankton |
| <i>AEC</i> | Aux | $assC_Zoo/ingC_Zoo$ | dl | AE in terms of C |
| <i>AEN</i> | Aux | $(assC_Zoo*NC_Zoo)/(ingC_Zoo*NC_Phy)$ | dl | AE in terms of N |
| <i>assC_Zoo</i> | Aux | {see Table 16.2} | gC gC ⁻¹ d ⁻¹ | Assimilation rate into zooplankton |
| <i>BRi</i> | Aux | {see Table 16.2} | gC gC ⁻¹ d ⁻¹ | Basal respiration that is met by respiration of excess C in diet |
| <i>DINr</i> | Aux | {see Table 16.3} | gN gC ⁻¹ d ⁻¹ | Zooplankton ammonium regeneration |
| <i>GGEC</i> | Aux | $(ingC_Zoo-voidC_Zoo-resC_Zoo-BRi)/ingC_Zoo$ | dl | GGE in terms of C |
| <i>GGEN</i> | Aux | $(ingC_Zoo*NC_Phy-voidN_Zoo-DINr)/(ingC_Zoo*NC_Phy)$ | dl | GGE in terms of N |
| <i>ingC_Zoo</i> | Aux | {see Table 16.2} | gC gC ⁻¹ d ⁻¹ | Ingestion rate of prey into zooplankton |
| <i>NC_Phy</i> | Aux | {see Table 15.1} | gN gC ⁻¹ | Phytoplankton N:C |
| <i>resC_Zoo</i> | Aux | {see Table 16.2} | gC gC ⁻¹ d ⁻¹ | Zooplankton respiration rate |
| <i>voidC_Zoo</i> | Aux | {see Table 16.3} | gC gC ⁻¹ d ⁻¹ | Voiding of C by zooplankton |
| <i>voidN_Zoo</i> | Aux | {see Table 16.3} | gN gC ⁻¹ d ⁻¹ | Voiding of N by zooplankton |

Table 16.4 Equations for Assimilation and Gross Growth Efficiencies. dl dimensionless.

16.9 Modifications to the Phytoplankton Model

The model developed in Chapter 15 needs a few modifications to account for removal of phytoplankton by zooplankton grazing, and return of ammonium from nutrient regeneration. These changes are indicated in Fig. 16.8, and detailed in Table 16.5.

Care needs to be taken when coupling models together to ensure all steps are included and that the units all align. The system balance needs to be updated and checked. Remember to set the dilution rate to zero for the test of system balance.

If you wished, you could also develop a system C variable as well. To do this, introduce a dissolved inorganic C (DIC) state variable, from which you need to drain DIC to support phytoplankton growth, and introduce DIC from zooplankton respiration. The value of what would then be *sysC* would then sum all the C-containing state variables.

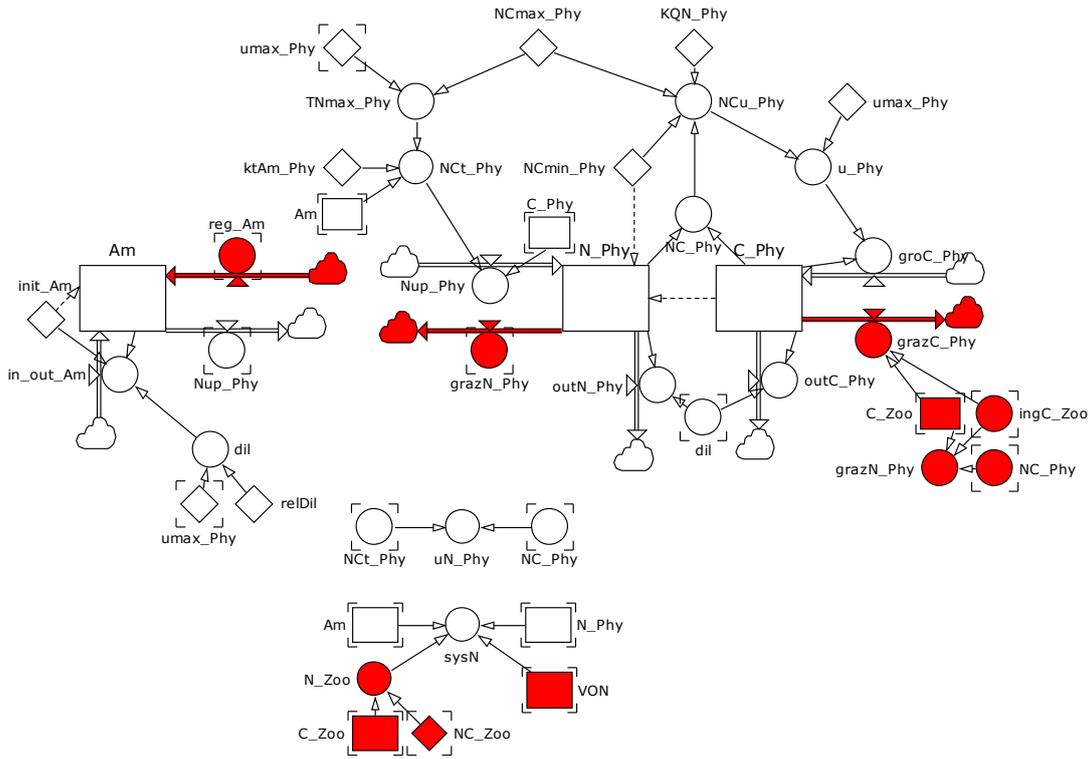


Fig. 16.8 The phytoplankton model developed in Chapter 15, showing in red the additions made to link this to the zooplankton model. See also Table 16.5.

| Variable | Type | Value | Unit | Description |
|------------------|------|--------------------------------|-------------------------------------|---|
| <i>C_Zoo</i> | SV | {see Table 16.1} | $\mu\text{gC L}^{-1}$ | Zooplankton C-biomass |
| <i>VON</i> | SV | {see Table 16.3} | $\mu\text{gN L}^{-1}$ | Faecal material -N |
| <i>NC_Zoo</i> | Con | 0.2 | gN gC^{-1} | N:C of zooplankton |
| <i>grazC_Phy</i> | Aux | $C_Zoo * ingC_Zoo$ | $\mu\text{gC L}^{-1} \text{d}^{-1}$ | Grazing upon phytoplankton population |
| <i>grazN_Phy</i> | Aux | $C_Zoo * ingC_Zoo * NC_Phy$ | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Grazing upon phytoplankton population in terms of N |
| <i>ingC_Zoo</i> | Aux | {see Table 16.2} | $\text{gC gC}^{-1} \text{d}^{-1}$ | Ingestion rate of prey into zooplankton |
| <i>N_Zoo</i> | Aux | $C_Zoo * NC_Zoo$ | $\mu\text{gN L}^{-1}$ | Zooplankton N-biomass |
| <i>NC_Phy</i> | Aux | {see Table 15.1} | gN gC^{-1} | N:C of phytoplankton |
| <i>reg_Am</i> | Aux | {see Table 16.3} | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Zooplankton population regeneration of ammonium |

Table 16.5 Additions to the phytoplankton model developed in Chapter 15.

16.10 Parameterising the Model

Conducting experiments on real predator-prey systems is fraught with difficulties, as already mentioned in Chapter 5. When trying to develop models to explore variable stoichiometry the challenges are greater again, not least because there is so much more to measure with all the ancillary logistic problems of sample size, separating organisms and faecal material, and analysis for (as here) both C and N.

Even under ideal conditions, some input variables would be extremely difficult to estimate. It is thus especially important to rationalise the model structure, to attempt to make it as realistic as possible in a generic sense, and to establish the best value for the “constants” through tuning the model against what data are available (see Chapter 14).

Building the model also makes the experimenter more aware of what data are needed. Most published works on consumer dynamics fail to report the nutritional value of the food, the nutrient history of the consumer, and the fate of materials that are not assimilated. And all too often they do not report variables in units of immediate use in support of modelling either.

Do not view this as a depressing state of affairs. It represents opportunities for new experimental approaches, ideally involving at the outset biologists who can build dynamic models to simulate the events.

16.11 Operating the Model

Some example model output is shown in Figs. 16.9, 10 & 11 using the input variables indicated. Note that the value of $sysN$ in these plots is not flat; re/Dil is not set at zero else the output is less interesting (there is a lesson there!) and hence the system is not in quasi equilibrium for the first 20-30 days.

Note also the interesting relationships between prey availability (C_{Phy}) with grazing ($ingC_{Zoo}$) and zooplankton growth (u_{Zoo}); this develops as a consequence of the dynamics of changing palatability of the prey ($palat_{Phy}$) as the whole system nutrient dynamics change.

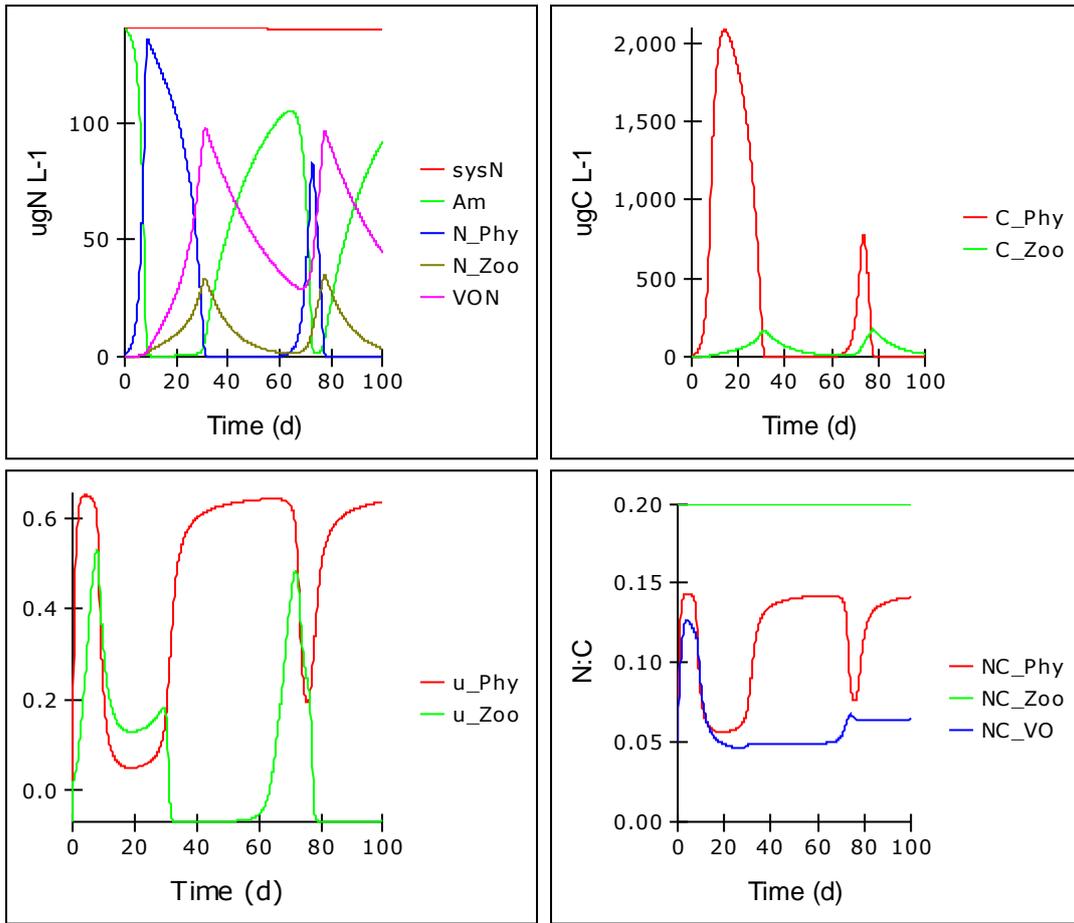


Fig. 16.9 Model output showing changes in N-based and C-based state variables, growth rates and N:C stoichiometry.

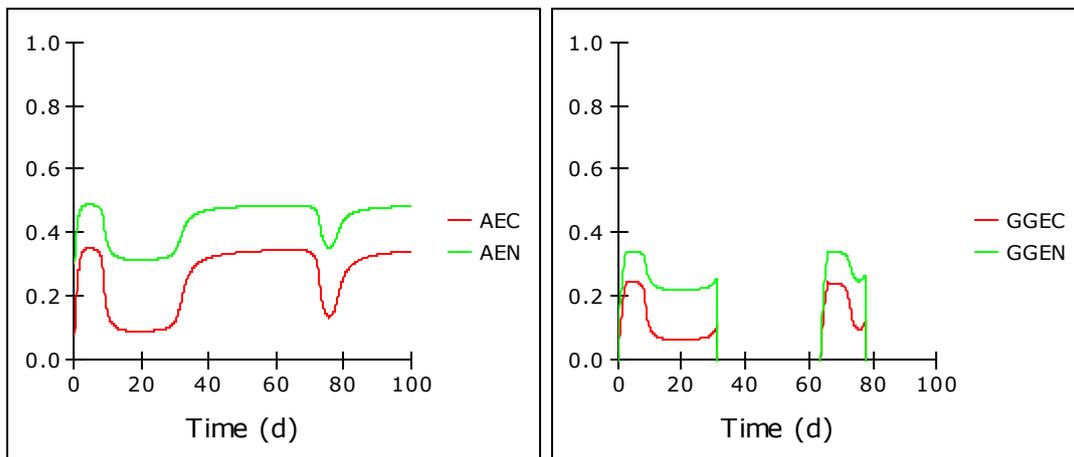


Fig. 16.10 Changes in C-based and N-based assimilation efficiency and gross growth efficiency for the model output in Fig. 16.9.

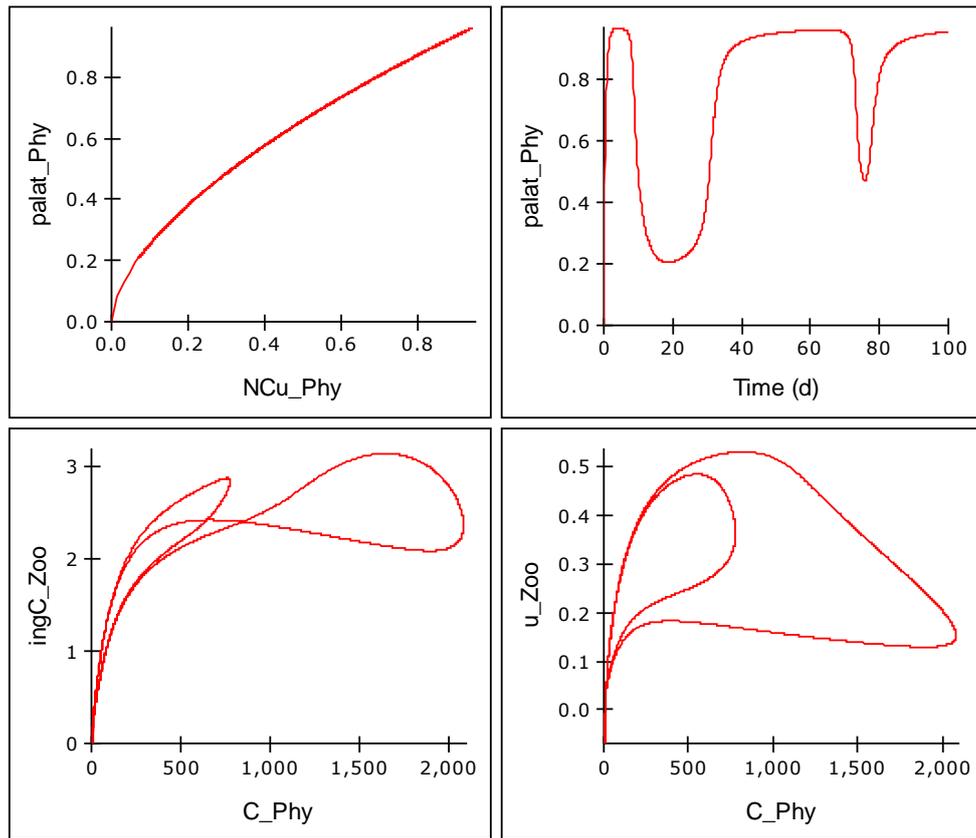


Fig. 16.11 Changes in palatability of the phytoplankton with nutrient status (NCu_Phy), and over time, and how in consequence the relationships between prey abundance (C_Phy), which is inversely related to nutrient status, affects ingestion and growth rates. The main dynamics are shown in Fig. 16.9.

16.12 Things to Explore

This model structure offers a multitude of opportunities to explore dynamic ecological stoichiometry. Below are just a few examples.

- i) With palatability and density dependent inefficiency disabled ($tox_Phy = 0$; $minAE_mult = 1$), see what effect altering the value of $NCmin_Phy$ has on the dynamics. Repeat with different nutrient loads and different values of $umax_Phy$ and $umax_Zoo$.
- ii) Try different values of tox_Phy , noting that this operates as a power function. You will see that altering the response curve for $palat_Phy$ has a very dramatic effect on the predator-prey interactions. If tox_Phy approaches 1 the system can suddenly generate a simulation of the formation of a **harmful algal bloom (HAB)**, or what would more appropriately be termed an **ecosystem disruptive algal bloom (EDAB)**. In essence, the phytoplankton grow to approaching nutrient exhaustion before predation can control it; once the phytoplankton are nutrient-stressed, and thus not palatable, the normal expected predator-prey dynamic fails (see Mitra & Flynn 2006b).

- iii) With $tox_Phy = 0$, explore the consequences of altering the impact of density dependent inefficiency (Flynn 2009), by altering $minAE_mult$ and $kGGT$. Look not only at the phytoplankton and zooplankton dynamics, but also at those of VOC and VON . In a real system, those voided organics would support trophic interactions in other parts of the ecosystem. Note how the value of N:C in the voided material (NC_VO) changes depending on the nutrient loading and hence the nutrient status of the phytoplankton when superfluous feeding occurs (AEC_Zoo is low).
- iv) You could also introduce a turnover function to recycle (degrade) VOC and VON (Chapter 5), or add a closure term on the zooplankton (Chapter 11).

16.13 Caveats

There are very many caveats to these types of models. Some particularly important ones are as follows:

- It is important to recall that the approach used here to configure the maximum grazing rate of the zooplankton is (as it was in Chapter 5) not that typically used; most modellers will set the maximum ingestion rate as a constant, and in consequence any changes in AE and respiration will erode the maximum growth rate even if food is available in excess. If you wish to follow such a route then you need to set $ingCmax_Zoo$ as a constant, using a value of AEC_Zoo commensurate with $Stoich_con = 1$, $AEquan = 1$. You will obtain very different dynamics, thus indicating if nothing else that the behaviour of the consumers in a food web, and our modelling of those consumers, is a critical determinant of dynamic ecology.
- There is no light-limitation functionality in the phytoplankton model; see Chapter 15, Section 15.7 (iv).
- There is only one predator-prey couple in the model. In reality there will be many more, not least because cannibalism within the zooplankton is to be expected. See Chapter 17.
- The usage of rectangular hyperbolic response curves to describe predation appears flawed (Flynn & Mitra 2016); it could be replaced with a form that better describes the curvi-linear nature of that response. This problem is in part a consequence of not explicitly considering organism numbers and size, both of which are of paramount importance in real ecology. This issue is explored in Chapter 17.

16.14 Where Next

To explore the dynamics of ecology further requires the building of more complex food webs. To do that you could easily build additional sub-models, each with different characteristics.

Aligning such characteristics will bring you into a sphere of ecological thinking associated with **trait-trade-offs**, the concept that to optimise one facet will inevitably cost with regards to another facet (see Flynn et al. 2015). The other feature that you will inevitably require is a description of resource selection, or preference. This applies both for inorganics (notably between ammonium vs nitrate for the support of phytoplankton growth), and especially for selection between different prey (see Mitra & Flynn 2006a, 2006b). In Chapter 17 we consider a food web with two phytoplankton species and a common predatory zooplankton.

17. Food Web Interactions: Allometry & Prey Selection

Terms and concepts introduced in this chapter- allometric scaling, encounter, motility, turbulence, (de)selection, satiation feedback

17.1 Ecological Context

So far we have considered very simple food chain interactions. In the real world, all organisms face choices between resources and, through a combination of biochemical, physiological and behavioural responses, they make their selections. But there is more to this than meets the eye and simulating different facets of the events is non-trivial. Behaviour of predators is also perhaps the factor that most attracts humans to observe organisms playing the survival game in the wild, or indeed in a test tube.

So, you are hungry - what will you do about it? Will you move around in search of food, and risk meeting your predator and being eaten up yourself? Will you try and eat anything you come across, that you bump into, or will you be picky? Will that pickiness vary depending on how hungry you are? What happens if your favourite food deteriorates in quality, perhaps even becoming noxious? How efficiently do you process your food? And what happens when you become satiated; do you sit there digesting your meal, or do you still race around chasing the next meal?

As before, while reference in what follows will be made to predator-prey systems, in most instances similar dynamics will occur in consumer-food interactions. The notable difference is of course that (dead) "food" is typically non-motile and will not struggle to escape!

We can split the processes into the following stages:

1. *Encountering the prey.* Predator and prey need to physically collide.
2. *Handling the prey.* Having collided, can the predator physically handle the prey? Is it the right size? Is it too powerful to restrain, so that it escapes? Is the predator satiated so that it does not need to capture the prey that it has collided with?
3. *Ingesting the prey.* Having captured the prey, does it taste right, or is it noxious?
4. *Digesting and assimilating the prey.* How does the quantity and quality of the food flowing through the gut, or being processed in food vacuoles, affect the subsequent dynamics of encounter-handling-ingesting? How does quality and quantity affect assimilation efficiency and the form of what is not assimilated?

We will work through these in turn, but before doing so it is worth noting how all of these processes interconnect. Fig. 17.1 gives a schematic, and its legend an explanation. The description that will be developed below does not pretend to do justice to the full complexity of reality, but it may at least (excuse the pun) provide food for thought.

An important feature of the model developed below concerns allometric (size-related) scaling. This is involved here in calculations of biomass vs numeric abundance, encounter rates, and motility. There are various "rules" that are commonly used that involve allometry. Classic "rules" relate higher maximum growth rates and also lower substrate half saturation constants as

features of smaller organisms. However, you should also be careful to consider the associated caveats. While size is most certainly important, there are also many other features of organisms that may mitigate or otherwise counter allometric rules. There are also features that may exacerbate the consequences of allometric scaling.

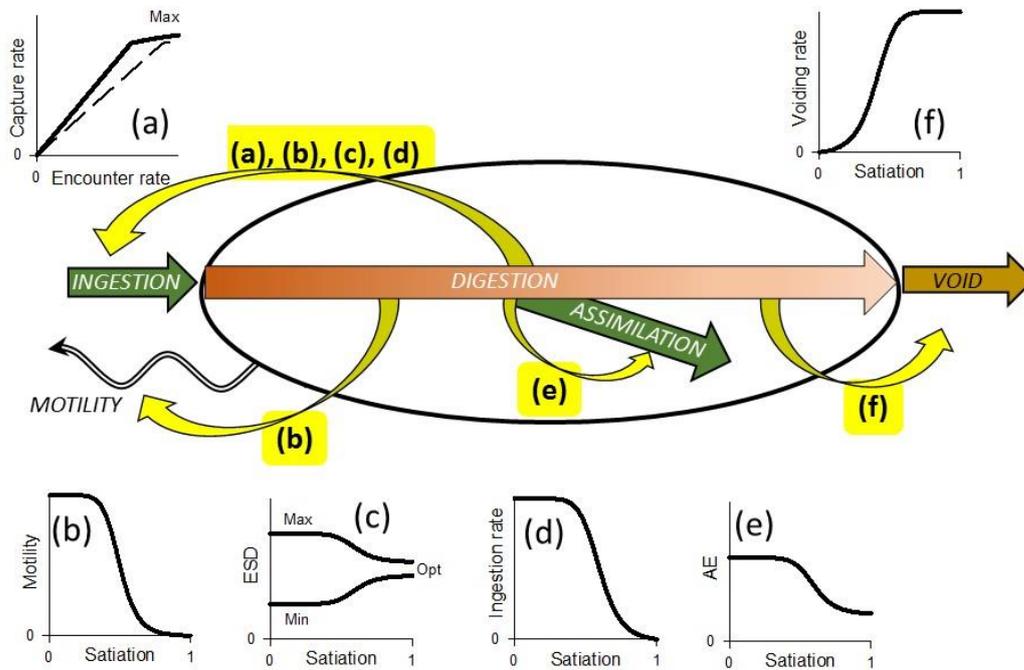


Fig. 17.1 Schematic showing range of interactions between prey (food) encounter, ingestion, digestion, assimilation and voiding. Yellow curved arrows indicate feedbacks; the sinusoidal arrow indicates consumer motility. Plot (a) shows the relationship between encounter and capture, which is initially linear but in the absence of any other feedbacks would be ultimately limited by handling at the point of capture or ingestion. The dashed line is for a prey type of lesser preference. Depending on preference, several prey items may be consumable over a period of time; consumption of any/all prey types contribute to satiation. Plot (b) shows satiation affecting motility, which in turn affects encounter rate (a). Set against this feedback is the need for some consumers to move for reasons other than feeding, and also that there may be motion of the prey relative to the consumer caused by their own motility and/or turbulence. Plot (c) shows how prey preference, indicated here by size selectivity, may be expected to tighten as satiation develops. Plot (d) shows how gut satiation itself also controls ingestion rate, effectively decreasing the maximum level (plateau value) of capture indicated in plot (a). Plot (e) shows assimilation efficiency declining with satiation, so that in the presence of abundant food digestion is less complete. Plot (f) shows how, especially in a peristaltic gut, satiation promotes voiding; this works with (e), to counter (d) to enhance the flow through of food. The relationship between prey abundance (per unit of space) and ingestion rate is an emergent property of all these interactions, coupled to other facets such as food quality and prior nutritional history of the consumer. From Flynn & Mitra (2016).

17.2 The Base Model

The basis for this model is that we developed in Chapter 16. That model comprised 1 phytoplankton and 1 zooplankton functional types. Here we now have two phytoplankton types, which we will term *Phy1* and *Phy2*. Each has state variables C_{Phy} and N_{Phy} describing carbon and nitrogen biomass. The phytoplankton model constructions are identical, except for the values of the constants that described critical traits (such as size, growth rate, toxicity etc.).

You could build sub-models using arrays. Using such an approach saves much coding effort, but here we will use a non-arrayed method, so we have for carbon biomass C_{Phy1} and C_{Phy2} . With an arrayed format we would have $C_{Phy}(i)$ where (*i*) takes an index number, here as 1, or 2; see Section 2.4.

17.3 Encountering Prey

Predators sense their prey through different methods; touch, chemical clue (scent), sight, fluid disturbance (noise or other pressure changes), or combinations thereof. In all instances there is a radius of perception. The most simple of these perceptions, and the one most obviously and directly linked to prey selection and actual capture, is touch. Touch is also the most appropriate perception mechanism for us to consider in the context of plankton.

The likelihood of colliding with a prey item depends on how large both the predator and the prey are, and the speeds of motion of both parties. Even if the predator is not moving (perhaps because with satiation it ceases all movement) a prey item may still collide with it. There are also the consequences of turbulence that may bring even non-motile predator and prey into contact.

The radius of perception will vary depending on the shape of the two organisms, and the presence of appendages such as feelers, but for simplicity we shall assume that the two organisms are spherical and that the radius of perception is thus also a function of the radius of the organisms themselves. It is convenient to refer to plankton size in terms of their equivalent spherical diameter (ESD); see Table 1.1 and its allied text in Chapter 1. The concept of ESD provides a route to compare organisms of different volume with respect to a single linear dimension; implicit in this calculation is an assumption that the organism shape is not too different from a sphere, an assumption that becomes increasingly questionable for larger metazoa (see also Fig. 1.1).

Motion of plankton through the water occurs through a combination of their own swimming or sedimentation, and also of turbulence. For the organisms themselves, we may assume ballistic motion; organisms are assumed to move in straight lines. In reality this very rarely happens, with organisms more likely describing what are termed “random walks” (or Lévy flights), combinations of ballistic movements or jumps, with periods of slower more random movements, or for smaller planktonic flagellates just spinning on the spot. Arguably, spinning on the spot increases the effective radius of perception, and certainly movement paths will impact on the likelihood of collision with other organisms or particles. Here, we just assume simple ballistic paths, as these serve, assuming homogeneous distribution of prey, to maximise encounters.

The encounter rate by a predator (Enc_s , prey predator⁻¹ s⁻¹) is described by Rothschild and Osborn (1988), with reference to organisms of stated size, as:

$$Enc_s = \pi (r_p + r_z)^2 \cdot N \cdot (v_p^2 + 3 \cdot v_z^2 + 4 \cdot w^2) \cdot (v_z^2 + w^2)^{-0.5} \cdot 3^{-1} \quad \text{Eq.17.1}$$

Here, the subscript p identifies the less motile of the organisms (usually the prey), subscript z the more motile organism (usually the predator), r is the organism radius (i.e., ESD/2; m), v is their respective speeds of motion (m s⁻¹), and N is numeric prey abundance (items m⁻³). The value of w describes the root-mean-squared turbulence (m s⁻¹); Rothschild and Osborn (1988) provide a relationship between wind speed and root-mean squared turbulence, considering values of w from 0 to 0.003 m s⁻¹, noting the relative importance of turbulence for encounters with smaller organisms.

It is important to recognise that we are considering encounters with reference to organism numeric abundance. Hitherto all our models have described organism abundance in terms of biomass.

The data summarised in Fig. 17.2 gives a relationship between organism size (ESD, data values ranging between 1.2 and 1900 μm) and motility (v , m s⁻¹) as described in Eq. 17.2.

$$v = 10^{-6} \cdot (38.542 \cdot ESD^{0.5424}) \quad \text{Eq.17.2}$$

It is interesting that at the larger sizes in Fig. 17.2 the speed in terms of body-lengths per second (plotted here as v/ESD) approaches the value of 3, which aligns with the cruising speed for a pelagic fish.

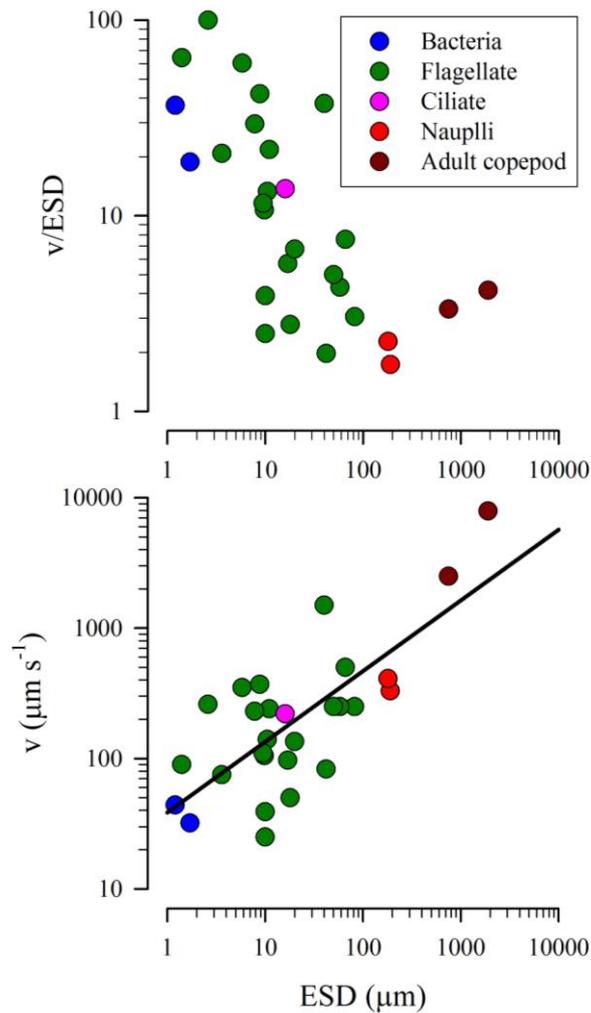


Fig. 17.2 Relationship between equivalent spherical diameter (*ESD*) and speed of motion (*v*). Data from Sommer (1988) and Visser & Kiørboe (2006). The line in the lower plot shows the line from Eq.17.2. Note the log scales. From Flynn & Mitra (2016).

The encounter rate per day (i.e., prey predator⁻¹ d⁻¹) is:

$$Enc_d = Enc_s \cdot 60 \cdot 60 \cdot 24 \quad \text{Eq.17.3}$$

To calculate organism numbers from the population biomass we need a relationship between organism size and C content. To do this we make use of the expressions developed by Straille (1997) and Menden-Deuer & Lessard (2000). These are illustrated in Fig. 17.3. We will make use of the “protist” relationship shown here.

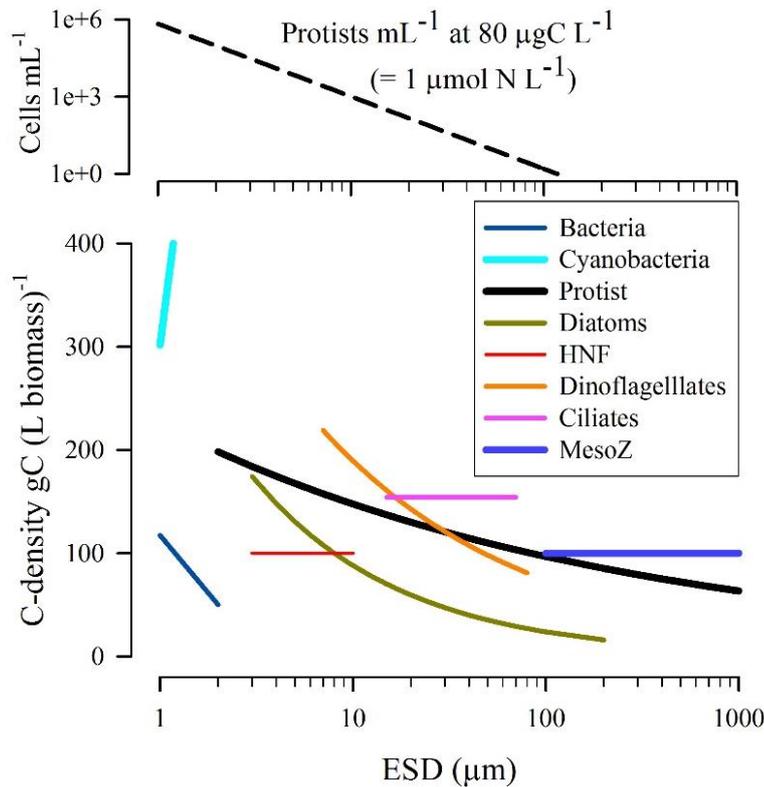


Fig. 17.3 Relationship between equivalent spherical diameter (ESD) and C-density within the biomass. Data reconfigured from Straile (1997) and Menden-Deuer & Lessard (2000). The upper plot shows the number of protist cells of different size (using the “Protist” relationship from the lower plot) per mL of suspension when those organisms are present at a population biomass of $80\mu\text{gC L}^{-1}$, which equates to $\sim 1\mu\text{mol biomass-N L}^{-1}$ assuming Redfield C:N for the prey. From Flynn & Mitra (2016).

The equation that we need is this:

$$C_{cell} = a \cdot cellVol^b \quad \text{Eq.17.4}$$

C_{cell} is pgC per cell, $cellVol$ is the cell volume in fL (i.e., μm^3), a and b are constants. The value of $cellVol$ is computed assuming spherical organisms (as $4/3 \cdot \pi \cdot r^3$, where radius r is $ESD/2$).

The sub-model for the encounter calculations is shown in Fig. 17.4, with the variables described in Table 17.1.

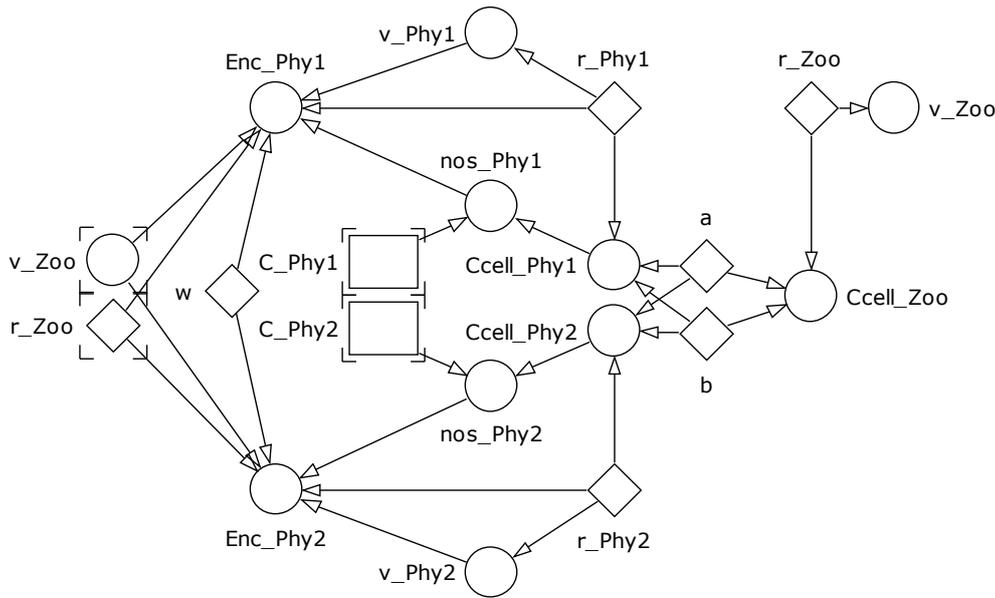


Fig. 17.4 Encounter sub-model. See also Table 17.1.

| Variable | Type | Value | Unit | Description |
|-------------------|------|--|--|--|
| <i>C_Phy1</i> | SV | {see Table 17.4} | µgC L ⁻¹ | Phy1 C-biomass |
| <i>C_Phy2</i> | SV | {see Table 17.4} | µgC L ⁻¹ | Phy2 C-biomass |
| <i>a</i> | Con | 0.216 | dl | Parameter for derivation of C-cell content for protist of a given volume |
| <i>b</i> | Con | 0.939 | dl | Parameter for derivation of C-cell content for protist of a given volume |
| <i>r_Phy1</i> | Con | 2.5 | µm | Radius of Phy1 cell |
| <i>r_Phy2</i> | Con | 5 | µm | Radius of Phy2 cell |
| <i>r_Zoo</i> | Con | 50 | µm | Radius of Zoo cell |
| <i>w</i> | Con | 0 | m s ⁻¹ | Root-mean-squared turbulence |
| <i>Ccell_Phy1</i> | Aux | $a^{*}(4/3*PI*(r_Phy1)^3)^b$ | pgC cell ⁻¹ | C content of Phy1 |
| <i>Ccell_Phy2</i> | Aux | $a^{*}(4/3*PI*(r_Phy2)^3)^b$ | pgC cell ⁻¹ | C content of Phy2 |
| <i>Ccell_Zoo</i> | Aux | $a^{*}(4/3*PI*(r_Zoo)^3)^b$ | pgC cell ⁻¹ | C content of Zoo |
| <i>Enc_Phy1</i> | Aux | $(24*60*60)*PI*(r_Phy1/1E6+r_Zoo/1E6)^2*nos_Phy1*(v_Phy1^2+3*v_Zoo^2+4*w^2)*((v_Zoo^2+w^2)^{-0.5})*3^{-1}$ | Phy1 Zoo ⁻¹ d ⁻¹ | Encounter rate of a cell of Phy1 by a cell of Zoo |
| <i>Enc_Phy2</i> | Aux | $(24*60*60)*PI*(r_Phy2/1E6+r_Zoo/1E6)^2*nos_Phy2*(v_Phy2^2+3*v_Zoo^2+4*w^2)*(v_Zoo^2+w^2)^{-0.5})*3^{-1}$ | Phy2 Zoo ⁻¹ d ⁻¹ | Encounter rate of a cell of Phy2 by a cell of Zoo |
| <i>nos_Phy1</i> | Aux | $10^9 * C_Phy1 / Ccell_Phy1$ | Phy1 cells m ⁻³ | Cell abundance of Phy1 |
| <i>nos_Phy2</i> | Aux | $10^9 * C_Phy2 / Ccell_Phy2$ | Phy2 cells m ⁻³ | Cell abundance of Phy2 |
| <i>v_Phy1</i> | Aux | $(10^{-6})*(38.542*(r_Phy1^2)^{0.5424})$ | m s ⁻¹ | Speed of motility of Phy1 |
| <i>v_Phy2</i> | Aux | $(10^{-6})*(38.542*(r_Phy2^2)^{0.5424})$ | m s ⁻¹ | Speed of motility of Phy2 |
| <i>v_Zoo</i> | Aux | $(10^{-6})*(38.542*(r_Zoo^2)^{0.5424})$ | m s ⁻¹ | Speed of motility of Zoo |

Table 17.1 Encounter sub-model variables. See Fig. 17.3.

17.4 Capturing the Prey

Having collided with the prey, the next question is whether this then results in capture. The viscosity of water at the scales of microplankton is akin to treacle for a human. The consequence is that as the predator “reaches out” for the prey the latter is pushed away. To secure contact some plankton deploy what amount to microscopic harpoons, termed trichocysts, or nematocysts (Gavelis et al. 2017). These projectiles are triggered by collision or proximal disturbance and results in delivery of a contractile filament that attaches to the prey so that it may be pulled into intimate contact with the predator and thence more likely ingested.

Different organisms are configured to optimally handle prey (food) of different types. While size is a critical component of “type” in this context, so are other features such as motility through which the prey may escape capture. Fig. 17.5 shows the relative size of phytoplankton prey for various predators. Some dinoflagellates attack organisms larger than themselves, but most predators consume prey that are relatively much smaller than themselves. Note that the relative size of prey is described in Fig. 17.5 in terms of ESD, while the nutritional value varies with ESD³ and varies again if the C-density of the organisms varies (see Fig. 17.3, and adjoining text). Panel (b) in Fig. 17.5 illustrates the consequence of different strategies in prey selection; if an organism is consuming small prey then the ingestion rate (as numbers of prey) needs to be many orders of magnitude faster to obtain the same nutritional input rate. Set against this is, of course, that for a given biomass abundance the numeric abundance may be orders of magnitude greater for smaller prey.

“Optimality” of prey size shown in Fig. 17.5 appears as a quotient, ranging from 0 to 1. This should not be confused with the probability of success in terms of capture. Even optimal prey may well not be captured every time; perhaps only 50% of encounters with such organisms may lead to capture. The forms of the optimality plots vary greatly between predators. The lower extreme may reflect a cut-off for particle handling, or that (for microflagellates) there are *de facto* simply no prey smaller than bacteria. The upper extreme may reflect an upper cut-off for particle handling or ingestion, and/or that larger prey are more likely to be able to escape capture due to their own motility. Aside from the aforementioned “harpoons”, prey may also be immobilised or indeed even killed or exploded by release of chemicals from the predator. Some dinoflagellates cast a veil over their prey, and essentially digest their prey externally. Whatever the mechanism in reality, somehow we need a response curve relating prey size to the likelihood of converting an encounter to a capture.

You could develop a response curve from data such as those used to generate Fig. 17.5 to describe prey size optimality. Alternatively you could go for something simpler, like a triangular distribution. Although this appears crude, it has the attraction that it is simple to manipulate with respect to the critical size limits setting the minimum (S_{min}), optimum (S_{op}), and maximum (S_{max}). Written using Boolean logic terms (which take the value 1 if true, and 0 if false), such a function looks like this:

$$PR=(S>S_{min})*(S<S_{max})*((S<S_{op})*(S-S_{min})/(S_{op}-S_{min})+(S>=S_{op})*(S_{max}-S)/(S_{max}-S_{op}))$$

Eq.17.5

Examples are shown in Fig. 17.6. The output proportional rate, PR , is multiplied by the encounter rate from Eq. 17.3.

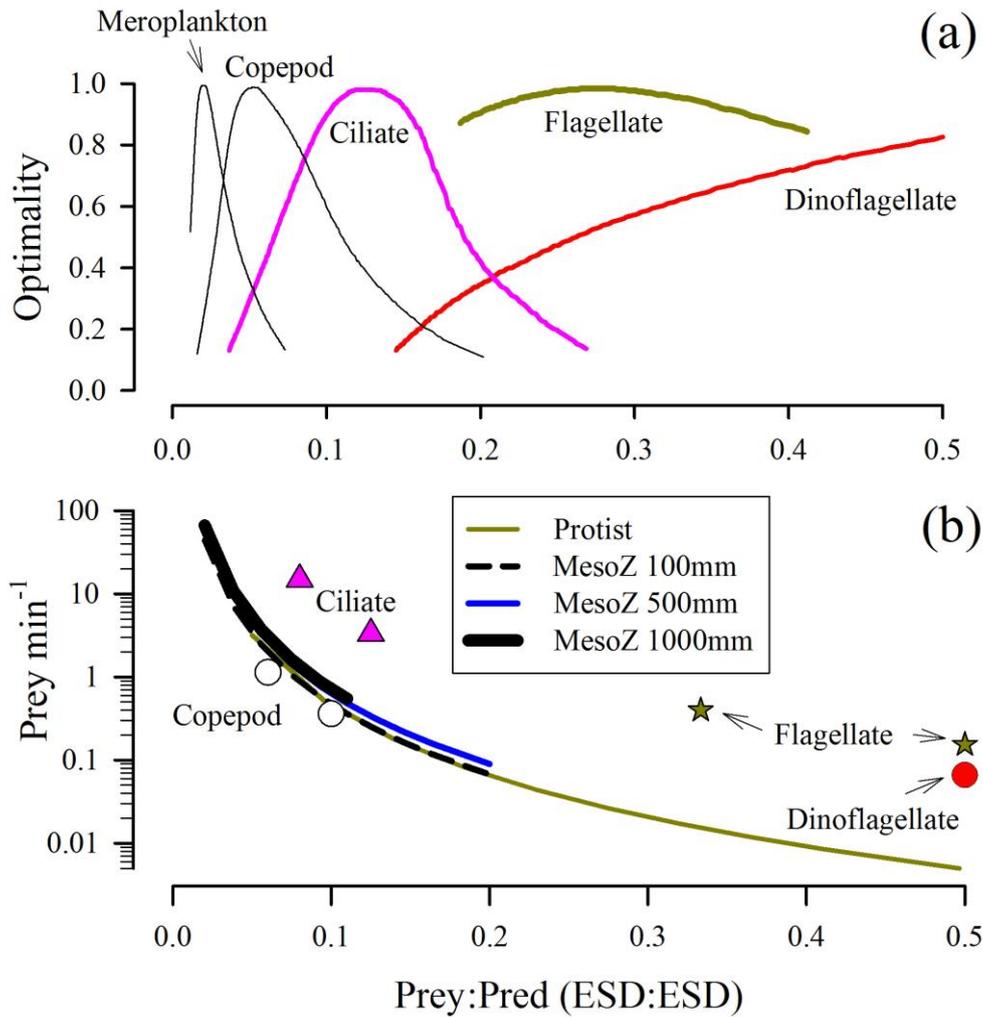


Fig. 17.5 Relationships between relative size of predator and optimal prey size (a) and prey capture rates required to attain a given C-specific rate of ingestion (b). Panel (a) is redrawn from Hansen et al. (1994); the dinoflagellate plot peaks at a size ratio of 1:1. Panel (b) shows, as lines, the required continual capture rate per minute to attain a day average ingestion rate of $1\text{g prey-C (g predator-C)}^{-1}\text{ d}^{-1}$. These values were computed through reference to the allometric relationships for protists and mesozooplankton shown in Fig. 17.3. Symbols show, as examples, maximum ingestion rates computed from relationships given in Hansen et al. (1997) for the organism types indicated. From Flynn & Mitra (2016).

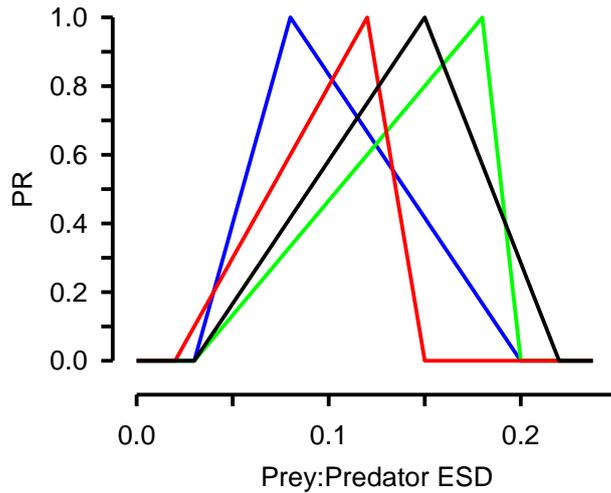


Fig. 17.6 Example triangular feeding optima response curves. The x-axis is of prey:predator sizes with respect to ESD, with the y-axis as the value of PR from Eq.17.5.

The sub-model for prey optimality is shown in Fig. 17.7 and the variables described in Table 17.2. Rather than using the Boolean equation format of Eq.17.5, in Table 17.2 an “IF” type of construct is used; you will need to use whichever equation construction is most appropriate for your modelling platform, being sure that it actually does what you intend it to do!

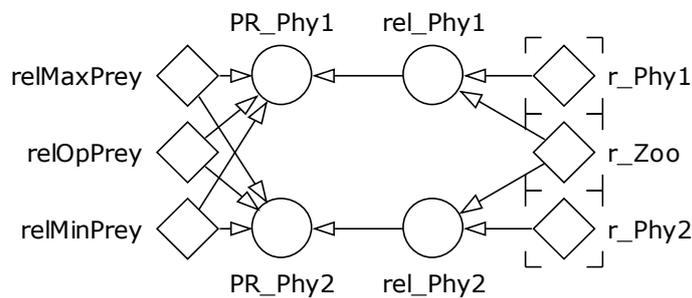


Fig. 17.7 Prey optimality sub-model. See also Table 17.2.

| Variable | Type | Value | Unit | Description |
|-------------------|------|--|------|---|
| <i>r_Phy1</i> | Con | {see Table 17.1} | µm | Radius of Phy1 cell |
| <i>r_Phy2</i> | Con | {see Table 17.1} | µm | Radius of Phy2 cell |
| <i>r_Zoo</i> | Con | {see Table 17.1} | µm | Radius of Zoo cell |
| <i>relMaxPrey</i> | Con | 0.3 | dl | Maximum prey:pred |
| <i>relMinPrey</i> | Con | 0.025 | dl | Minimum prey:pred |
| <i>relOpPrey</i> | Con | 0.2 | dl | Optimal prey:pred |
| <i>PR_Phy1</i> | Aux | IF((<i>relMaxPrey</i> > <i>rel_Phy1</i> AND <i>rel_Phy1</i> > <i>relMinPrey</i>),IF(<i>rel_Phy1</i> < <i>relOpPrey</i> ,(<i>rel_Phy1</i> - <i>relMinPrey</i>)/(<i>relOpPrey</i> - <i>relMinPrey</i>),(<i>relMaxPrey</i> - <i>rel_Phy1</i>)/(<i>relMaxPrey</i> - <i>relOpPrey</i>)),0) | dl | Prey handling index for Phy1, taking into account the prey:pred relative size |
| <i>PR_Phy2</i> | Aux | IF((<i>relMaxPrey</i> > <i>rel_Phy2</i> AND <i>rel_Phy2</i> > <i>relMinPrey</i>),IF(<i>rel_Phy2</i> < <i>relOpPrey</i> ,(<i>rel_Phy2</i> - <i>relMinPrey</i>)/(<i>relOpPrey</i> - <i>relMinPrey</i>),(<i>relMaxPrey</i> - <i>rel_Phy2</i>)/(<i>relMaxPrey</i> - <i>relOpPrey</i>)),0) | dl | Prey handling index for Phy2, taking into account the prey:pred relative size |
| <i>rel_Phy1</i> | Aux | <i>r_Phy1</i> / <i>r_Zoo</i> | dl | prey:pred for Phy1 |
| <i>rel_Phy2</i> | Aux | <i>r_Phy2</i> / <i>r_Zoo</i> | dl | prey:pred for Phy2 |

Table 17.2 Prey optimality sub-model variables. See Fig. 17.7.

17.5 Palatability and Ingestion

Thus far, for a given single prey-predator couple, we could compute the relationship between prey abundance and capture rate offline and just introduce the resultant constant into the model. However, when we consider multiple prey items with changes in nutritional value we have the added complexity of palatability as well as differential rates of encounter all set against satiation. Changes in nutritional status may also often be associated with changes in organism size.

If the prey item does not taste right then it will be rejected; most logically rejection will occur at the point of contact rather than post-ingestion. There are examples of rejection (egestion) after ingestion, and indeed of protists “learning” not to ingest unpalatable prey (Flynn et al. 1996). In an environment where encounters with inert particles (such as clay) may be common, routine rejection of particles that are of the correct size for capture but are not nutritious may be expected.

Palatability can also change for a specific prey item, such that a species which is of good food quality is eaten, while if it becomes a poor food quality item then it is rejected. We may suspect that prey that is itself nutritionally stressed (deprived of N or P) will be of lesser value to a predator on account of not only having a poor elemental (C:N:P) composition, but because that status likely is associated with a poor balance in fatty acid and amino acid types, and also in the accumulation of noxious secondary metabolites. We have considered this issue before, in Chapter 16, noting that food quality may not vary in a linear fashion with elemental stoichiometry.

To introduce the subject of food quality it is easiest to work with a quotient describing palatability, with 1 indicating optimal quality, and 0 complete rejection. We can use the approach given in Section 16.4, and now combine it with Eqs. 17.3 & 17.5. This gives us a potential rate of ingestion of a particular prey type accounting for encounter (*Enc_Phy*), prey handling (*PR_Phy*) and palatability (*palat_Phy*). In addition we assign a quotient describing the capture potential for the

optimal prey (*Optimal_CR*); this defines the greatest likelihood of a capture event succeeding. In total, we have this:

$$CR_Phy = Enc_Phy * PR_Phy * palat_Phy * Optimal_CR \quad \text{Eq.17.5}$$

This gives us the potential capture rate for the phytoplankton, as *CR_Phy*. Why “potential” and not actual? Because irrespective of all else, any consumer can only consume so much at a time. So now we need to relate the potential ingestion of different prey types to the level of satiation of the predator.

17.6 Satiation Feedback Modulating Ingestion

The cumulative ingestion of any and all prey items over the recent past controls satiation, and hence whether more ingestion can occur. The process is more complex than this though, because the more a consumer ingests, typically the more rapidly the material flows through the digestive system and the lower the efficiency with which it is processed. That is to say that the gut transit time (or its equivalent for food vacuole in a protist) decreases, and so does the assimilation efficiency; see Fig. 17.1.

The previous sections describe the potential capture rate of a particular prey type in consequence of size, motility, scope for capture, and palatability. At low prey abundance, and with all else constant, as described by the model there is thus a linear relationship between abundance and ingestion rate. At the upper extreme, ingestion rate must saturate as a function of satiation; we can expect that saturation event to be curvilinear so we need an approach to merge the linear and saturation phases. Furthermore, while each prey type may be considered to be handled essentially as a separate entity (note the typically brief handling time in Fig. 17.5), the collective recently ingested biomass contributes to satiation. We also need to consider that while particles are handled at ingestion, satiation is a function of biomass, not of particle count per se.

So, first we need to convert the particle-specific ingestion rate (*CR_Phy*, from Eq.17.5) into a biomass-specific rate. We do that using the converse of the relationship we used earlier to convert biomass to numbers (Eq.17.4) for both the prey and the predator. This gives us the potential C-specific capture rate, *CRC_Phy* (Fig. 17.8; Table 17.3).

Let the potential biomass-specific rate of capture for prey *i* be *Cp_i*. The total biomass-specific ingestion rate, *I* (Eq.17.6), is a minimum function of the total possible capture rates (sum *Cp_i*) and a curvilinear function that empirically describes a feedback on ingestion from satiation through reference to a half-saturation constant for the biomass ingestion rate of all prey items (*K_I*), and the maximum biomass-specific ingestion rate (*I_{max}*, d⁻¹).

$$I = MIN \left(I_{max} \cdot \frac{\sum Cp_i}{\left(\sum Cp_i + K_I \right)}, \sum Cp_i \right) \quad \text{Eq.17.6}$$

Satiation feedback on ingestion is thus controlled by the half-saturation constant K_i , with higher values resulting in the feedback developing earlier. It should be noted that K_i is associated with the total ingestion rate and thence with satiation; it is not referenced to external prey abundance and hence there is no variable in this whole model description equivalent to the K_{pred} term used in all of our previous descriptions of predator-prey interactions (e.g. Chapter 16). The default value for K_i is given as $\frac{1}{4}$ of the maximum ingestion rate (see Flynn & Mitra 2016).

In terms of the model that we are building, Eq.17.6 looks like this:

$$ingC_Zoo = \text{MIN}(ingCmax_Zoo * SCRC / (SCRC + KI), SCRC) \quad \text{Eq.17.7}$$

where the sum of the potential capture rates, $SCRC$, is given as:

$$SCRC = CRC_Phy1 + CRC_Phy2 \quad \text{Eq.17.8}$$

Now we have the actual total ingestion rate, as well as the potential capture rates for each prey, we compute the actual predation rate for each prey simply by proportion. The ingestion rate of the i^{th} prey type is thus given as I_i (Eq.17.9).

$$I_i = I \cdot \frac{Cp_i}{\sum Cp_i} \quad \text{Eq.17.9}$$

Thus for Phy1:

$$ingPhy1C = ingC_Zoo * CRC_Phy1 / SCRC \quad \text{Eq.17.10}$$

And finally, because we need to know the nutritional value of the total diet, we need to compute the N:C of $ingC_Zoo$ ($ingNC$). This again we do by proportion of the rates of ingestion of the individual prey types (CRC_Phy) and their N:C values (NC_Phy). Thus:

$$ingNC = (CRC_Phy1 * NC_Phy1 + CRC_Phy2 * NC_Phy2) / SCRC \quad \text{Eq.17.11}$$

The complete prey capture sub-model is shown in Fig. 17.8, with variables described in Table 17.3.

If there were more prey types, then additional potential and actual capture (ingestion) rates would be required, and the above equations modified accordingly.

Importantly, this model describes changes in “prey preference”. The structure allows for the de-selection of prey due to changes in toxicity or nutritional status. Ingestion of other prey types is only increased in proportion as allowed by encounter kinetics and satiation feedback. It is also possible for all prey types to be de-selected. Many models cannot describe such kinetics; see Mitra & Flynn (2006a, 2006b) and Flynn & Mitra (2016) for further discussion.

17.7 Phytoplankton, Zooplankton, Voiding and Ammonium Sub-models

The rest of the model is built in an analogous fashion to that in Chapter 16. For completeness the slightly modified sub-models and the descriptions of their variables are given in Figs. 17.9 – 17.12, and Tables 17.4 – 17.7.

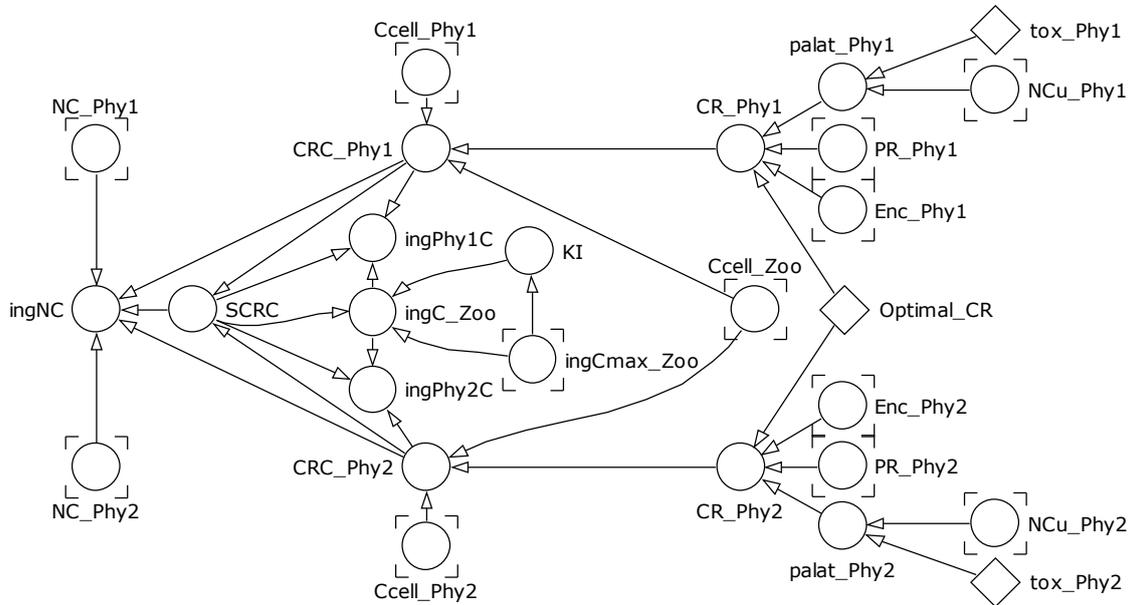


Fig. 17.8 Prey capture sub-model. See Table 17.3.

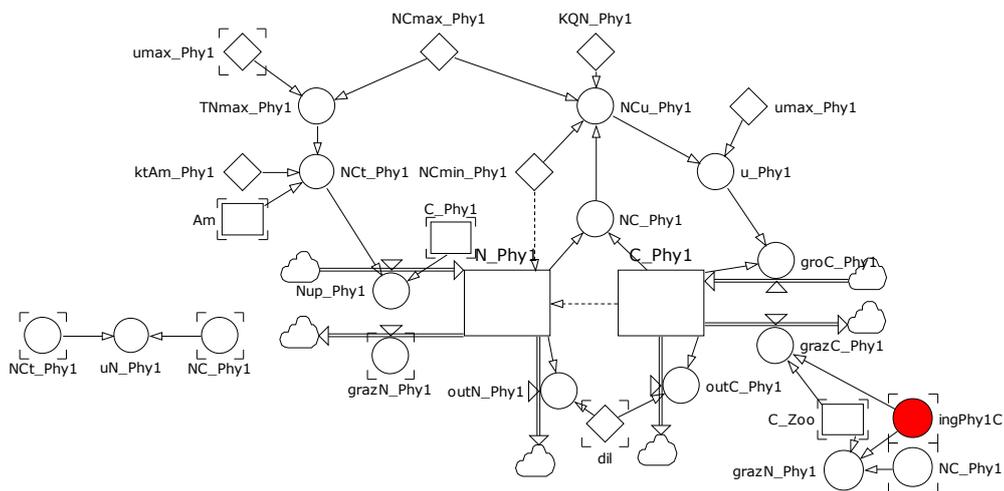


Fig. 17.9 Phy1 sub-model. The sub-model for Phy2 has the exact same structure, just with “Phy1” changed to “Phy2”. See Table 17.4. The only functional difference from the phytoplankton model described in Chapter 16 is indicated by the red variable.

| Variable | Type | Value | Unit | Description |
|-------------------|------|---|--|---|
| <i>Optimal_CR</i> | Con | 1 | dl | proportion of prey of optimal characteristics captured by starved Zoo |
| <i>tox_Phy1</i> | Con | 0 | dl | Toxicity factor for Phy1; 0 not toxic |
| <i>tox_Phy2</i> | Con | 1.1 | dl | Toxicity factor for Phy2 |
| <i>CR_Phy1</i> | Aux | $Enc_Phy1 * PR_Phy1 * palat_Phy1 * Optimal_CR$ | Phy1 Zoo ⁻¹ d ⁻¹ | potential capture of Phy1 taking into account all factors |
| <i>CR_Phy2</i> | Aux | $Enc_Phy2 * PR_Phy2 * palat_Phy2 * Optimal_CR$ | Phy2 Zoo ⁻¹ d ⁻¹ | potential capture of Phy2 taking into account all factors |
| <i>CRC_Phy1</i> | Aux | $CR_Phy1 * Ccell_Phy1 / Ccell_Zoo$ | gC gC ⁻¹ d ⁻¹ | Potential C-specific ingestion of Phy1 |
| <i>CRC_Phy2</i> | Aux | $CR_Phy2 * Ccell_Phy2 / Ccell_Zoo$ | gC gC ⁻¹ d ⁻¹ | Potential C-specific ingestion of Phy2 |
| <i>Enc_Phy1</i> | Aux | {see Table 17.1} | Phy1 Zoo ⁻¹ d ⁻¹ | encounter rate of a cell of Phy1 by a cell of Zoo |
| <i>Enc_Phy2</i> | Aux | {see Table 17.1} | Phy2 Zoo ⁻¹ d ⁻¹ | encounter rate of a cell of Phy2 by a cell of Zoo |
| <i>ingC_Zoo</i> | Aux | $MIN(ingCmax_Zoo * SCRC / (SCRC + KI), SCRC)$ | gC gC ⁻¹ d ⁻¹ | Ingestion rate of prey into zooplankton |
| <i>ingNC</i> | Aux | $(CRC_Phy1 * NC_Phy1 + CRC_Phy2 * NC_Phy2) / SCRC$ | gN gC ⁻¹ | N:C of incoming food |
| <i>ingPhy1C</i> | Aux | $ingC_Zoo * CRC_Phy1 / SCRC$ | gC gC ⁻¹ d ⁻¹ | ingestion rate of Phy1 by Zoo |
| <i>ingPhy2C</i> | Aux | $ingC_Zoo * CRC_Phy2 / SCRC$ | gC gC ⁻¹ d ⁻¹ | ingestion rate of Phy2 by Zoo |
| <i>KI</i> | Aux | $ingCmax_Zoo / 4$ | gC gC ⁻¹ d ⁻¹ | satiation control constant |
| <i>NC_Phy1</i> | Aux | N_Phy1 / C_Phy1 | g N gC ⁻¹ | N:C quota for Phy1 |
| <i>NC_Phy2</i> | Aux | N_Phy2 / C_Phy2 | gN gC ⁻¹ | N:C quota for Phy2 |
| <i>NCu_Phy1</i> | Aux | $((1 + KQN_Phy1) * (NC_Phy1 - NCmin_Phy1)) / ((NC_Phy1 - NCmin_Phy1) + KQN_Phy1 * (NCmax_Phy1 - NCmin_Phy1))$ | dl | Quotient for N-status of Phy1 |
| <i>NCu_Phy2</i> | Aux | $((1 + KQN_Phy2) * (NC_Phy2 - NCmin_Phy2)) / ((NC_Phy2 - NCmin_Phy2) + KQN_Phy2 * (NCmax_Phy2 - NCmin_Phy2))$ | dl | Quotient for N-status of Phy2 |
| <i>palat_Phy1</i> | Aux | $(NCu_Phy1 + 1e-6)^{tox_Phy1}$ | dl | Palatability index for Phy1 |
| <i>palat_Phy2</i> | Aux | $(NCu_Phy2 + 1e-6)^{tox_Phy2}$ | dl | Palatability index for Phy2 |
| <i>PR_Phy1</i> | Aux | $IF((relMaxPrey > rel_Phy1 AND rel_Phy1 > relMinPrey), IF((rel_Phy1 < relOpPrey), (rel_Phy1 - relMinPrey) / (relOpPrey - relMinPrey), (relMaxPrey - rel_Phy1) / (relMaxPrey - relOpPrey)), 0)$ | dl | Prey handling index for Phy1 |
| <i>PR_Phy2</i> | Aux | $IF((relMaxPrey > rel_Phy2 AND rel_Phy2 > relMinPrey), IF((rel_Phy2 < relOpPrey), (rel_Phy2 - relMinPrey) / (relOpPrey - relMinPrey), (relMaxPrey - rel_Phy2) / (relMaxPrey - relOpPrey)), 0)$ | dl | Prey handling index for Phy2 |
| <i>SCRC</i> | Aux | $CRC_Phy1 + CRC_Phy2$ | gC gC ⁻¹ d ⁻¹ | sum of potential prey capture rates |

Table 17.3 Prey capture sub-model variables. See Fig. 17.8.

| Variable | Type | Value | Unit | Description |
|-------------------|------|---|--------------------------------------|--|
| <i>Am</i> | SV | {see Table 17.7} | μg N L ⁻¹ | Ammonium-N |
| <i>C_Phy1</i> | SV | 12 <i>+groC_Phy1</i> <i>-grazC_Phy1</i> <i>-outC_Phy1</i> | μg C L ⁻¹ | Phy1 C-biomass |
| <i>N_Phy1</i> | SV | <i>C_Phy1*NCmin_Phy1</i> <i>+Nup_Phy1</i> <i>-grazN_Phy1</i> <i>-outN_Phy1</i> | μg N L ⁻¹ | Phy1 N-biomass |
| <i>dil</i> | Con | {see Table 17.7} | d ⁻¹ | Dilution rate |
| <i>KQN_Phy1</i> | Con | 10 {Phy2 version = 10} | dl | KQ for N-quota |
| <i>ktAm_Phy1</i> | Con | 14 {Phy2 version = 70} | μg N L ⁻¹ | Half saturation constant for Am transport |
| <i>NCmax_Phy1</i> | Con | 0.15 {Phy2 version = 15} | gN gC ⁻¹ | Maximum N:C |
| <i>NCmin_Phy1</i> | Con | 0.07 {Phy2 version = 0.05} | gN gC ⁻¹ | Minimum N:C |
| <i>umax_Phy1</i> | Con | 0.5 {Phy2 version = 0.8} | g C gC ⁻¹ d ⁻¹ | Maximum C-specific growth rate |
| <i>grazC_Phy1</i> | Aux | <i>C_Zoo*ingPhy1C</i> | ugC L ⁻¹ d ⁻¹ | Loss of phytoplankton C-biomass by grazing |
| <i>grazN_Phy1</i> | Aux | <i>C_Zoo*ingPhy1C*NC_Phy1</i> | ugN L ⁻¹ d ⁻¹ | Loss of phytoplankton N-biomass by grazing |
| <i>groC_Phy1</i> | Aux | <i>C_Phy1*u_Phy1</i> | μgC L ⁻¹ d ⁻¹ | Growth rate in phytoplankton-C |
| <i>NC_Phy1</i> | Aux | <i>N_Phy1/C_Phy1</i> | gN gC ⁻¹ | Phytoplankton N:C quota |
| <i>NCT_Phy1</i> | Aux | <i>TNmax_Phy1*Am/(Am+ktAm_Phy1)</i> | gN gC ⁻¹ d ⁻¹ | Phytoplankton C-specific N transport rate |
| <i>NCu_Phy1</i> | Aux | $((1+KQN_Phy1)*(NC_Phy1-NCmin_Phy1))/((NC_Phy1-NCmin_Phy1)+KQN_Phy1*(NCmax_Phy1-NCmin_Phy1))$ | dl | Quotient for N-status |
| <i>Nup_Phy1</i> | Aux | <i>C_Phy1*NCT_Phy1</i> | μgN L ⁻¹ d ⁻¹ | Phytoplankton population uptake of ammonium-N |
| <i>outC_Phy1</i> | Aux | <i>C_Phy1*dil</i> | μgC L ⁻¹ d ⁻¹ | Washout of C_Phy |
| <i>outN_Phy1</i> | Aux | <i>N_Phy1*dil</i> | μg N L ⁻¹ d ⁻¹ | Washout of N_Phy |
| <i>TNmax_Phy1</i> | Aux | <i>umax_Phy1*NCmax_Phy1</i> | gN gC ⁻¹ d ⁻¹ | Maximum C-specific N-transport rate |
| <i>u_Phy1</i> | Aux | <i>umax_Phy1*NCu_Phy1</i> | gC gC ⁻¹ d ⁻¹ | C-specific growth rate controlled by N:C quota |
| <i>uN_Phy1</i> | Aux | <i>NCT_Phy1/NC_Phy1</i> | g N gN ⁻¹ d ⁻¹ | N-specific growth rate |

Table 17.4 Phy1 sub-model variables. The sub-model for Phy2 has the exact same structure, just with variable names “Phy1” changed to “Phy2”. Note the alternative values for constants for the Phy2 version. See Fig. 17.9. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

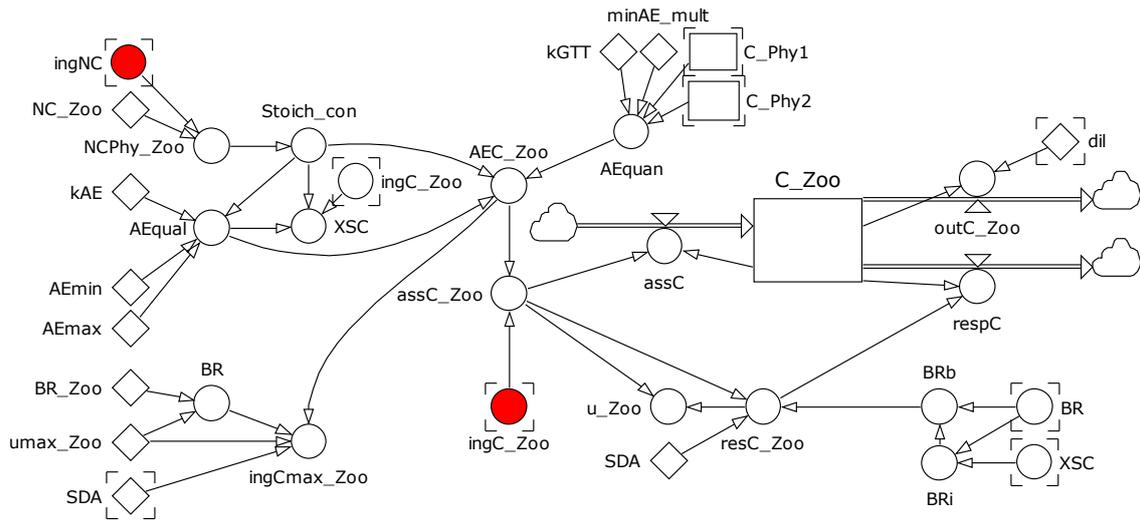


Fig. 17.10 Zooplankton sub-model. See Table 17.5. The differences from the zooplankton model described in Chapter 16 are indicated by red variables.

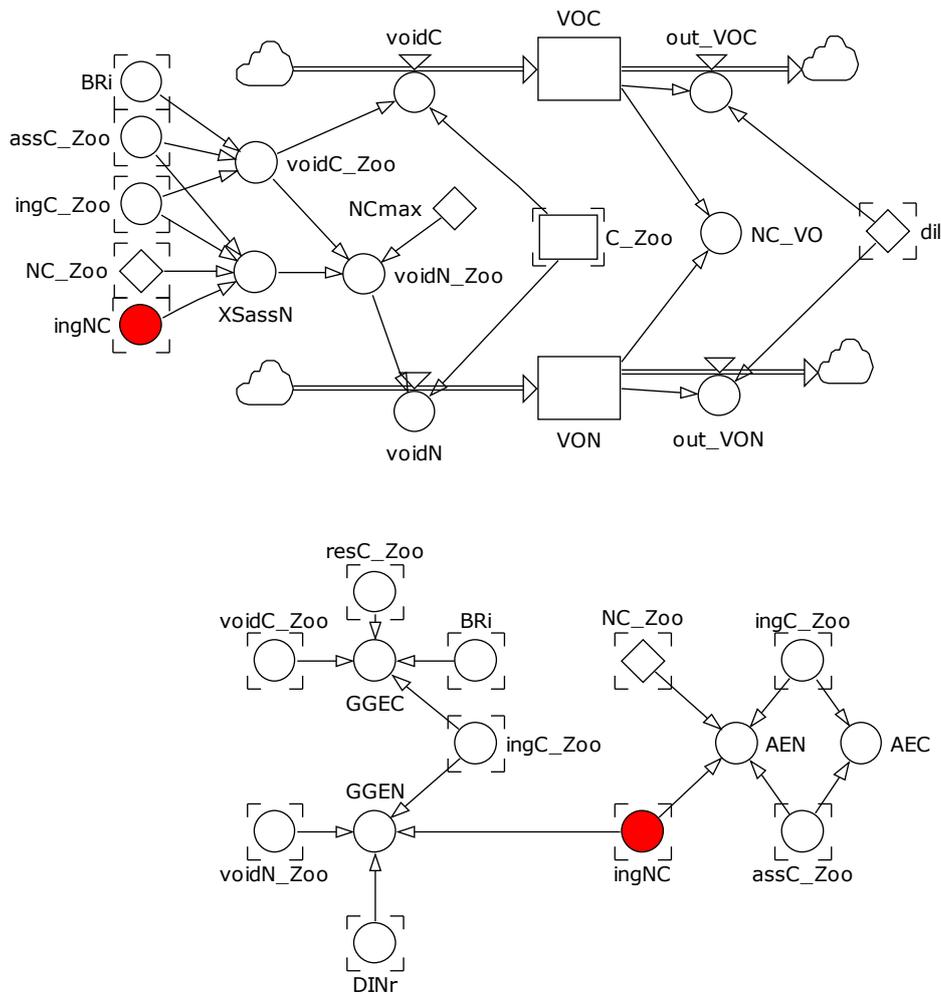


Fig. 17.11 Voiding and efficiency sub-models. See Table 17.6. The differences from the model described in Chapter 16 are indicated by red variables.

| Variable | Type | Value | Unit | Description |
|--------------------|------|--|-------------------------------------|---|
| <i>C_Phy1</i> | SV | {see Table 17.4} | µg C L ⁻¹ | Phy1 C-biomass |
| <i>C_Phy2</i> | SV | {see Table 17.4} | µg C L ⁻¹ | Phy2 C-biomass |
| <i>C_Zoo</i> | SV | 1 + <i>assC</i> - <i>outC_Zoo</i> - <i>respC</i> | µg C L ⁻¹ | Zoo C-biomass |
| <i>AEmax</i> | Con | 0.6 | dl | maximum AE for N |
| <i>AEmin</i> | Con | 0.2 | dl | minimum AE for N |
| <i>BR_Zoo</i> | Con | 0.1 | dl | Basal respiration as a proportion of <i>umax_Zoo</i> |
| <i>dil</i> | Con | {see Table 17.7} | d ⁻¹ | Dilution rate |
| <i>kAE</i> | Con | 1.00E+03 | dl | Constant for control of AE in response to prey quality |
| <i>kGTT</i> | Con | 100 | ugC L ⁻¹ | Curve control for density dependant inefficiency |
| <i>minAE_mult</i> | Con | 1 | dl | Minimum AE-C scalar for density dependant inefficiency |
| <i>NC_Zoo</i> | Con | 0.2 | gN gC ⁻¹ | N:C of zooplankton |
| <i>SDA</i> | Con | 0.3 | dl | Specific Dynamic Action |
| <i>umax_Zoo</i> | Con | 0.693 | d ⁻¹ | Zoo maximum C-specific growth rate |
| <i>AEC_Zoo</i> | Aux | <i>Stoich_con</i> * <i>AEEqual</i> * <i>AEquan</i> | dl | Operational AE for C |
| <i>AEEqual</i> | Aux | $\frac{AEmin+(AEmax-AEmin)*Stoich_con}{(Stoich_con+kAE)*(1+kAE)}$ | dl | efficiency parameter for assimilation |
| <i>AEquan</i> | Aux | $\frac{(1-minAE_mult)*(1-C_Phy1/(C_Phy1+kGTT))+minAE_mult}{C_Zoo*assC_Zoo}$ | dl | AE-C scalar for density dependant inefficiency |
| <i>assC</i> | Aux | <i>C_Zoo</i> * <i>assC_Zoo</i> | ugC L ⁻¹ d ⁻¹ | C-assimilation into Zoo biomass |
| <i>assC_Zoo</i> | Aux | <i>AEC_Zoo</i> * <i>ingC_Zoo</i> | gC gC ⁻¹ d ⁻¹ | Zoo C-specific assimilation rate |
| <i>BR</i> | Aux | <i>umax_Zoo</i> * <i>BR_Zoo</i> | d ⁻¹ | Zoo basal respiration |
| <i>BRb</i> | Aux | <i>BR</i> - <i>BRi</i> | gC gC ⁻¹ d ⁻¹ | BR not met from dietary excess C |
| <i>BRi</i> | Aux | IF(<i>BR</i> <= <i>XSC</i> , <i>BR</i> , <i>XSC</i>) | gC gC ⁻¹ d ⁻¹ | BR met from dietary excess C |
| <i>ingC_Zoo</i> | Aux | {see Table 17.3} | gC gC ⁻¹ d ⁻¹ | Ingestion rate of prey-C |
| <i>ingCmax_Zoo</i> | Aux | $(umax_Zoo*(1+SDA)+BR)/AEC_Zoo$ | gC gC ⁻¹ d ⁻¹ | Maximum ingestion rate |
| <i>ingNC</i> | Aux | {see Table 17.3} | gN gC ⁻¹ | N:C of incoming food |
| <i>NCPhy_Zoo</i> | Aux | <i>ingNC/NC_Zoo</i> | dl | ratio of diet N:C to predator N:C |
| <i>outC_Zoo</i> | Aux | <i>C_Zoo</i> * <i>dil</i> | ugC L ⁻¹ d ⁻¹ | Washout of zooplankton biomass |
| <i>resC_Zoo</i> | Aux | <i>BRb</i> + <i>assC_Zoo</i> * <i>SDA</i> | gC gC ⁻¹ d ⁻¹ | Zooplankton respiration rate |
| <i>respC</i> | Aux | <i>C_Zoo</i> * <i>resC_Zoo</i> | ugC L ⁻¹ d ⁻¹ | Zooplankton population respiration |
| <i>SCRC</i> | Aux | {see Table 17.3} | gC gC ⁻¹ d ⁻¹ | sum of potential prey capture rates |
| <i>Stoich_con</i> | Aux | MIN(<i>NCPhy_Zoo</i> ,1) | dl | Selection of release of N related to difference in food to consumer N:C |
| <i>u_Zoo</i> | Aux | <i>assC_Zoo</i> - <i>resC_Zoo</i> | d ⁻¹ | Zooplankton growth rate |
| <i>XSC</i> | Aux | IF(<i>Stoich_con</i> <1, <i>AEEqual</i> * <i>ingC_Zoo</i> *(1- <i>Stoich_con</i>),0) | gC gC ⁻¹ d ⁻¹ | C available for digestion but not used for protoplasmic purposes. |

Table 17.5 Zooplankton sub-model. See Fig. 17.10. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

| Variable | Type | Value | Unit | Description |
|------------------|------|---|-------------------------------------|--|
| <i>C_Zoo</i> | SV | {see Table 17.5} | $\mu\text{g C L}^{-1}$ | Zoo C-biomass |
| VOC | SV | 0 +voidC -out_VOC | $\mu\text{g C L}^{-1}$ | Faecal material -C |
| VON | SV | 0 +voidN -out_VON | $\mu\text{g N L}^{-1}$ | Faecal material -N |
| <i>dil</i> | Con | {see Table 17.7} | d^{-1} | dilution rate |
| <i>NC_Zoo</i> | Con | {see Table 17.3} | gN gC^{-1} | N:C of zooplankton |
| <i>NCmax</i> | Con | 0.3 | gN gC^{-1} | maximum mass ratio of N:C attainable in organic form |
| <i>AEC</i> | Aux | $\text{assC_Zoo}/\text{ingC_Zoo}$ | dl | AE in terms of C |
| <i>AEN</i> | Aux | $(\text{assC_Zoo} * \text{NC_Zoo}) / (\text{ingC_Zoo} * \text{NC_Phy1})$ | dl | AE in terms of N |
| <i>BRi</i> | Aux | {see Table 17.5} | $\text{gC gC}^{-1} \text{d}^{-1}$ | BR met from dietary excess C |
| <i>DINr</i> | Aux | {see Table 17.7} | $\text{gN gC}^{-1} \text{d}^{-1}$ | Zooplankton ammonium regeneration |
| <i>GGEC</i> | Aux | $(\text{ingC_Zoo} - \text{voidC_Zoo} - \text{resC_Zoo} - \text{BRi}) / \text{ingC_Zoo}$ | dl | GGE in terms of C |
| <i>GGEN</i> | Aux | $(\text{ingC_Zoo} * \text{NC_Phy1} - \text{voidN_Zoo} - \text{DINr}) / (\text{ingC_Zoo} * \text{NC_Phy1})$ | dl | GGE in terms of N |
| <i>ingC_Zoo</i> | Aux | {see Table 17.3} | $\text{gC gC}^{-1} \text{d}^{-1}$ | Ingestion rate of prey-C |
| <i>ingNC</i> | Aux | {see Table 17.3} | gN gC^{-1} | N:C of incoming food |
| <i>N_Zoo</i> | Aux | {see Table 17.7} | $\mu\text{gN L}^{-1}$ | Zooplankton N-biomass |
| <i>NC_VO</i> | Aux | VON/VOC | gN gC^{-1} | N:C of voided organics |
| <i>out_VOC</i> | Aux | $\text{VOC} * \text{dil}$ | $\mu\text{gC L}^{-1} \text{d}^{-1}$ | Washout of voided C |
| <i>out_VON</i> | Aux | $\text{VON} * \text{dil}$ | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Washout of voided N |
| <i>resC_Zoo</i> | Aux | {see Table 17.5} | $\text{gC gC}^{-1} \text{d}^{-1}$ | Zooplankton respiration rate |
| <i>voidC</i> | Aux | $\text{C_Zoo} * \text{voidC_Zoo}$ | $\mu\text{gC L}^{-1} \text{d}^{-1}$ | Population rate of C voiding |
| <i>voidC_Zoo</i> | Aux | $\text{ingC_Zoo} - \text{assC_Zoo} - \text{BRi}$ | $\text{gC gC}^{-1} \text{d}^{-1}$ | Voiding of C by zooplankton |
| <i>voidN</i> | Aux | $\text{C_Zoo} * \text{voidN_Zoo}$ | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Population rate of N voiding |
| <i>voidN_Zoo</i> | Aux | $\text{IF}((\text{XSassN}/\text{voidC_Zoo} > \text{NCmax}), \text{voidC_Zoo} * \text{NCmax}, \text{XSassN})$ | $\text{gN gC}^{-1} \text{d}^{-1}$ | Voiding of N by zooplankton |
| <i>XSassN</i> | Aux | $\text{ingC_Zoo} * \text{ingNC} - \text{assC_Zoo} * \text{NC_Zoo}$ | $\text{gN gC}^{-1} \text{d}^{-1}$ | Amount of N initially in the organic form to be voided to maintain constant predator N:C |

Table 17.6 Voiding and efficiency sub-model variables. See Fig. 17.11. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

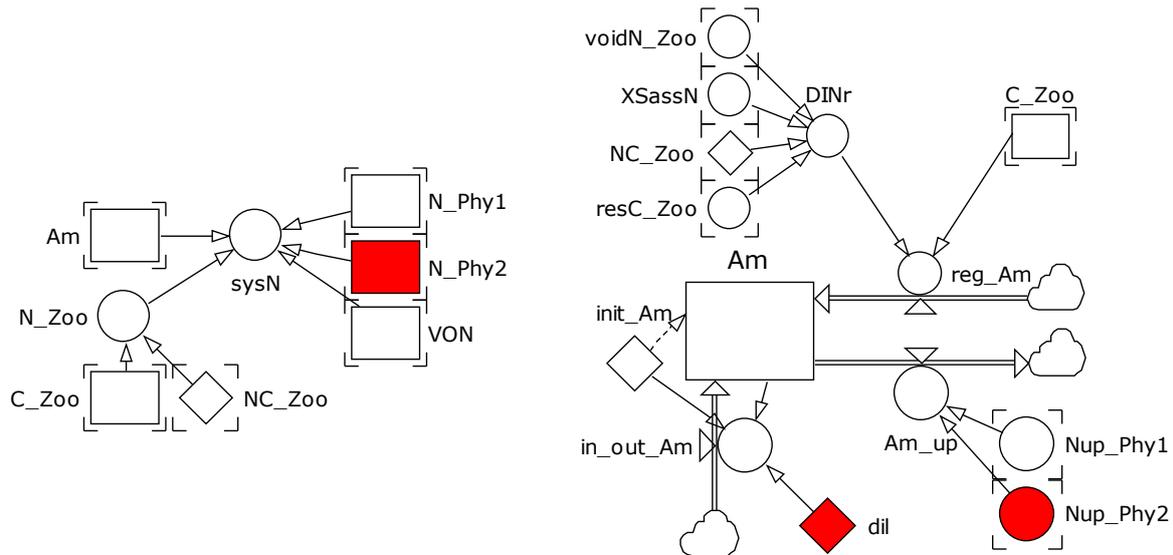


Fig. 17.12 Ammonium and system-N sub-models. See Table 17.7. The differences from the model described in Chapter 16 are indicated by red variables.

| Variable | Type | Value | Unit | Description |
|------------------|------|--|--------------------------------------|--|
| <i>Am</i> | SV | <i>init_Am</i> <i>+in_out_Am</i> <i>+reg_Am</i> <i>-Am_up</i> | $\mu\text{g N L}^{-1}$ | Ammonium-N |
| <i>C_Zoo</i> | SV | {see Table 17.5} | $\mu\text{g C L}^{-1}$ | Zooplankton C-biomass |
| <i>N_Phy1</i> | SV | {see Table 17.4} | $\mu\text{g N L}^{-1}$ | Phy1 phytoplankton-N |
| <i>N_Phy2</i> | SV | {see Table 17.4} | $\mu\text{g N L}^{-1}$ | Phy2 phytoplankton-N |
| <i>VON</i> | SV | {see Table 17.6} | $\mu\text{g N L}^{-1}$ | Faecal material -N |
| <i>dil</i> | Con | 0.05 | d^{-1} | Dilution rate |
| <i>init_Am</i> | Con | 280 | $\mu\text{g N L}^{-1}$ | Input ammonium-N |
| <i>NC_Zoo</i> | Con | {see Table 17.5} | gN gC^{-1} | N:C of zooplankton |
| <i>Am_up</i> | Aux | <i>Nup_Phy1+Nup_Phy2</i> | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | total consumption of ammonium |
| <i>in_out_Am</i> | Aux | <i>dil*(init_Am-Am)</i> | $\mu\text{g N L}^{-1} \text{d}^{-1}$ | nutrient exchange |
| <i>Nup_Phy1</i> | Aux | {see Table 17.4} | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Phy1 phytoplankton population uptake of ammonium-N |
| <i>Nup_Phy2</i> | Aux | {see Table 17.4} | $\mu\text{gN L}^{-1} \text{d}^{-1}$ | Phy2 phytoplankton population uptake of ammonium-N |
| <i>resC_Zoo</i> | Aux | {see Table 17.5} | $\text{gC gC}^{-1} \text{d}^{-1}$ | Zooplankton respiration rate |
| <i>voidN_Zoo</i> | Aux | {see Table 17.6} | $\text{gN gC}^{-1} \text{d}^{-1}$ | Voiding of N by zooplankton |
| <i>XSassN</i> | Aux | {see Table 17.6} | $\text{gN gC}^{-1} \text{d}^{-1}$ | Amount of N initially in the organic form to be voided to maintain constant predator N:C |

Table 17.7 Ammonium and system-N sub-model variables. See Fig. 17.12. The values for state variables are for the initial numeric value, and (in red) for the flows in (+) and out (-) of the state variable.

17.8 Parameterising the Model

Other than matters already described in Chapter 16 (Section 16.10), this model requires information on the size of the organisms, their speed or motility and (if of interest) turbulence. As you may wish to consider in Section 17.10, size and motility of organisms may also vary significantly with nutritional status.

17.9 Operating the Model

Some example model output is shown in Figs. 17.13 and 17.14 using the input variables indicated in the tables of variables given in this chapter. The disparity between encounter and ingestion rates (Fig. 17.14) is due to differences in cell size between Phy1 and the larger cell sized Phy2. Phy2 has a higher maximum growth rate, but a poorer half saturation for ammonium coupled with a lower NC_{min} and a level of toxicity that develops when it becomes N-stressed. Ultimately, in this simulation, Phy2 loses out even though its realised growth rate is similar (Fig. 17.13), as it is of a size more suited to capture by the zooplankton. Also as ammonium regeneration occurs, the N-status of Phy2 improves and hence its toxicity declines. If the ammonium load (set by *init_Am*) is lower, however, a totally different story develops (not shown – try it!).

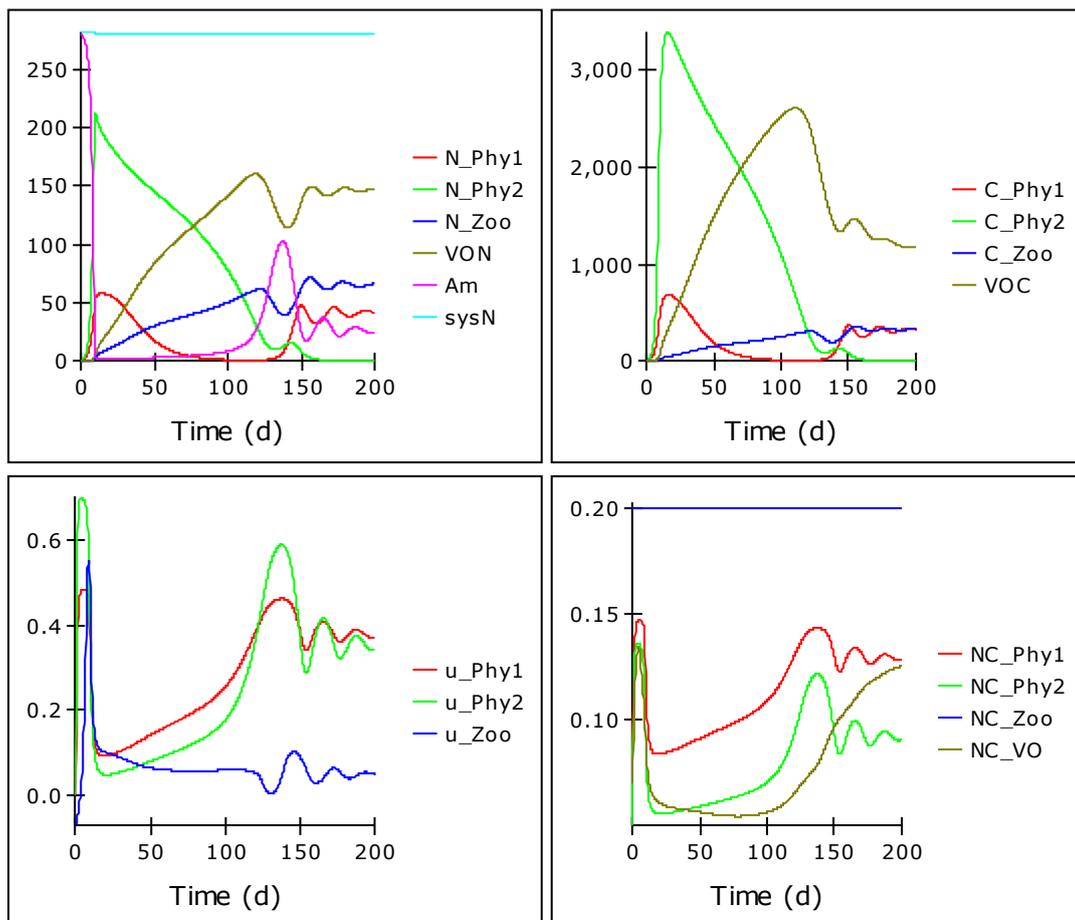


Fig. 17.13 Example model output, showing changes in C and N biomass, growth rates and the N:C of the components. See also Fig. 17.14.

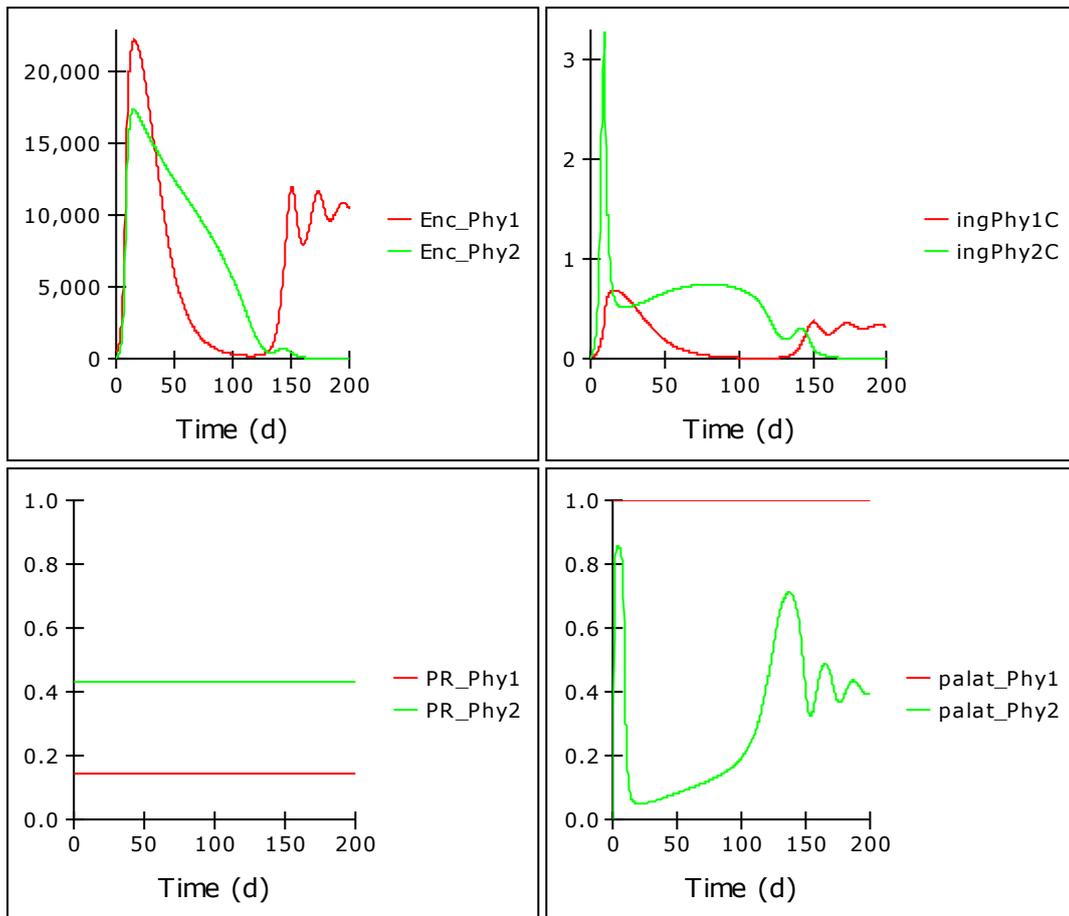


Fig. 17.14 Changes in encounter rates (Enc), ingestion (ing), relative optimality for predation (PR) and palatability (palat) for phytoplankton Phy1 and Phy2. See also Fig. 17.13.

17.10 Things to Explore

Even more than with the model developed in Chapter 16, this model structure offers a multitude of opportunities to explore dynamic stoichiometric ecology. Below are just a few suggestions.

- i. Change *init_Am* and/or introduce a light-limitation sub-model and mixing depth.
- ii. Change the kinetics for *Am* transport and/or growth rates of different components.
- iii. Change the radius of the phytoplankton cells with nutrient status. Typically a N or light-limited phytoplankton is smaller, while a P-stressed cell is larger and they also tend to clump together (perhaps in consequence they then escape capture all together – but is that good for the nutritional status of the individual, as nutrient regeneration from zooplankton activity ceases! See Mitra & Flynn 2006b).
- iv. Alter toxicity, the NC quota range and kinetics of ammonium transport into the phytoplankton. You may wish to consider how these, and light-limitation (which is brought on by self-shading in dense cell suspensions at high nutrient loading) are all connected.
- v. Make the motility of zooplankton relate to satiation. You could do this by reference to the ratio of zooplankton growth rate relative to its maximum.
- vi. Change the radius of the zooplankton with satiation. You may well expect a satiated zooplankton to be larger (as well as slower).

- vii. Enact *AE_quan*, and/or replace the current crude description with a satiation-linked mechanism. Again, you could do this by relating satiation to the rate of zooplankton growth relative to its maximum.
- viii. Introduce turbulence (vary *w*) – see Rothschild and Osborn (1988).
- ix. Altering the shape of the prey optimality description. You could trade-off the breadth of prey capture optimisation (*relminPrey* to *relmaxPrey*) against the value of *Optimal_CR*.

17.11 Caveats

There are again very many caveats to these types of models. Some particularly important ones are as follows:

- As for the models described in Chapters 15 & 16, the lack of light limitation enacted here is an important omission. Where there is light limitation nutrient limitation is less likely so while phytoplankton growth rates are lower, the nutrient status is higher. See Section 15.7 (vi).
- Motion is assumed to be ballistic, and rates of motion do not change with satiation. There are various issues here; these are expanded upon in Flynn & Mitra (2016).
- No changes in prey or predator size with nutrient status are considered. Changes in size affect the likelihood of encounters (assuming speed is unaffected) and also the nutritional content of the encountered prey.
- No relationship is included between the breadth of prey optimisation and the likelihood of a successful capture. You may expect that an optimal prey-predator evolution would see a narrowing of the breadth of prey capture potential but with enhanced capture success.
- Lack of allelopathic interactions between prey. Allelopathy and other chemical-mediated interactions between organisms, can be an important factor in phytoplankton-phytoplankton interactions. A failure to correctly describe such interactions can result in a failure of the model to simulate reality (Mitra & Flynn 2006a, 2006b).

17.12 Where Next

This is the last chapter in this book that develops a model. To explore the dynamics of ecology further requires the building of yet more complex food webs, and/or to better describe additional traits of the component organisms. And then there is whole issue of changes in the physico-chemical environment to consider (some of which are functions of biological activity, but most are not).

18. Concluding Comments

By the time you have reached this point you should have built and played with a good few models; “played” because hopefully you should have found the whole process engaging and enjoyable, as well as educational. Through that process you will have also modified models, building in additional functions, or perhaps started your own constructs from scratch. You will have learnt something about what works and what does not, and how to fix what is broken.

Albert Einstein said that: *Scientists investigate that which already is; engineers create that which has never been.*

Models are creations, and modellers bring some level of engineering to life sciences. Some models may appear so conceptual that they are not representative of real biological systems, but even the most complex models remain (by definition) simplifications of reality.

This phrase, “simplification of reality”, could seem to a biologist as an excuse for omitting what they may view as details of critical importance. In this context, there is a sharp contrast between molecular biology (evermore detail, evermore divisions between organisms) and systems biology/ecology modelling (which requires the merging of physiological processes, the formation of functional groups containing different species, genera or even phyla). Another sharp contrast, I suggest, is that biologists “own” molecular biology, while “ownership” of modelling tends to lay with mathematicians and allied scientists.

Modelling undertaken by the average biologist is mainly limited to statistics. Few physiologists, people who have actually worked in experimental laboratories, develop and use dynamic models. And that, to my mind, represents a significant loss to science. Most biologists or ecologists would likely not even be able to identify major flaws in a modelling paper, even if they looked for them. (Not that peer review of a modelling paper is easy, even for an expert.) Ironically, they may be willing to believe the results (especially when presented in a high profile journal, or conference) and quote them in support of their own interests, without appreciating the limitations of the underlying modelling science.

The origins of this book rest in my experience that students of biology and ecology can easily engage with modelling if they have the right tools. And many enjoy it. What these students do not enjoy is modelling using simple abstractions that they view as being, well, too abstract. That is why the first models in this book are specifically not Logistic and Lotka-Volterra models. Students also (like us all) want to see results of some form sooner rather than later. I do not believe that teaching one unknown (here, dynamic modelling) through another unknown (computer coding, such as R, C, Fortran etc.) is the best way to proceed. The learning curves for both these skills is steep with many pitfalls along the way. Hence my use of a graphic user interface (GUI) platform.

As an algal physiologist by PhD, I entered simulation modelling as a biologist, with a view to including in my models aspects of physiology that I perceived as being of greatest importance. When I started I asked my mentor, Mike Fasham, whether I should develop models in Fortran or stick to using a GUI platform (then, Powersim Constructor). “Absolutely stick to the GUI platform!” was the response. The point was that to develop a model that could do justice to the biology we were interested in (ammonium-nitrate interactions in phytoplankton), Mike argued that the last thing that I needed was a fight with the coding platform.

Traditionally modellers often deploy what is described (albeit, not actually with total regard to its origins) as “Occam’s razor”; *only include that which is important*. Judging what is really important is difficult. And this brings us to another comparison with engineering. Engineers typically over-engineer their constructions, to provide redundancy and safety. Only after much research are structures simplified, making them lighter, more efficient to manufacture, etc. By analogy, one could argue that modellers of life sciences should work from complex-to-simple.

Most biologists, biochemists and ecologists are familiar with making flow diagrams and similar visual representations. Making conceptual models that are complex is not a problem for the average ecophysiologicalist. However, having to answer all those question marks in the Forrester diagram was a salutary experience; it reminded me of how little we know with any certainty. And it also enforced upon my subsequent experiment designs an underlying ethos to collect data that were amendable to the systems modelling process. As biologists and ecologists we do know more than enough to realise that judging how to “*only include that which is important*” is non-trivial. For sure the final model in this book (Chapter 17) appear complex; to many it may appear extremely complex. Yet, if you have worked through from Chapter 4, I hope that you will be as likely to be concerned about what is missing from that final model as much as with its complexity.

The complex-to-simple concept is in diametric conflict with the way that many modellers apply their interpretation of Occam’s razor. Rather than assuming that we know which processes are of least importance, such that we do not even bother including them in models, the complex-to-simple approach seeks to justify simplifications by testing for redundancy. It may be useful to keep this in mind as you develop your own models.

I will leave you with a suggested correction to an oft-misused quote:

*All **statistical** models are wrong, but some are useful.* (modified, after George Box)

And my own version, directed specifically at simulation models of dynamic ecology:

All simulation models are incomplete, but they should not be wrong.

Finally, a quote from the mathematician and biologist, Jacob Bronowski:

Science is the acceptance of what works and the rejection of what does not. That needs more courage than we might think.

Good luck!

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