14 Modelling considerations

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14.1 Introduction

Numerical models can be viewed as a simplified representation of the real world. They comprise a system of rules that are combined with a number of initial conditions (e.g. nutrient distribution) and boundary conditions (e.g. atmospheric forcing) to make inferences about the state of affairs. A very similar procedure takes place when interpreting observations or planning experiments: the readings of instruments are translated following a set of rules into biogeochemically relevant properties; these are then arranged into a coherent picture in the mind of the scientist. Numerical models require that the rules be represented in a formal mathematical description, which has, at least in theory, the advantage of a clear and unambiguous language that should help to make models transparent and portable between different investigators. Another advantage is that the numerical model formulation requires the quantitative comparison of different parts of the system. Conceptual models developed from empirical or phenomenological considerations can take us only so far, and we often learn considerably more about the system when quantitative comparisons of, say, the balance of terms for an element do not agree.

Numerical models can be used to put data of different quality, isolated in space and in time, into a coherent context. This process can benefit from the concept of data assimilation that aims at a most efficient combination of information contained in the data with information contained in the model's rules. However, the complex theoretical and operational apparatus of data assimilation has, so far, limited its application. Probably the most widespread applications of numerical models are to explore logical consequences of hypotheses ("what if" experiments) and to identify sensitivities of integral properties to individual processes. The former category includes scenario simulation into the future. An important point to make about models is that, with a few exceptions, they cannot make predictions or insights about phenomenon that are not at some level included in the set of rules defining the model equations. In this respect models are intimately tied to laboratory and field work. The "what if" scenarios are only as good as the set of rules, and these scenarios typically are working on known (if only poorly) processes.

Numerical models can basically address the same kind of scientific questions as other scientific methods. In this respect, models are just another tool, comparable to, for example, mass spectrometry. However, models have a unique ability to firstly test our synthesised understanding of a given system and secondly extrapolate in time or space to regions where data is sparse. Calibrated model results can identify problems with our underlying conceptual understanding and highlight observational and experimental needs. Further, models can identify the perturbation envelope for experimental activities, for example pH and Ω ranges, and identify sensitive areas (e.g. the Arctic). Model results can also contribute to the identification of new hypotheses that require testing by data. Consequently, scientists who develop and apply models should not be viewed as potential "end-users" of experiments or observational campaigns. Models, as well as field and laboratory experiments should rather be designed in conjunction with each other, building on the strengths of the different techniques.

Predictive models are, in general, one of the key methods for synthesising understanding into a format usable by decision- and policymakers. Indeed, the recent emergence of climate change as a mainstream issue, which depends to a large extent on climate model scenario simulations, has enabled the far more rapid recognition of ocean acidification as a parallel concern for policymakers. Consequently, the scientific community is being challenged to produce robust and relevant science that underpins international policy development on a relatively short timescale. However, whilst prediction of the carbonate system response is reasonably robust (e.g. Caldeira & Wickett, 2003; Orr *et al.,* 2005), predicting the response of ecosystems and resources is problematic and is at a very early stage (for example Blackford & Gilbert, 2007; Bourret *et al.,* 2007; Hashioka & Yamanaka, 2007). This is due in part to the complexity of system drivers and in part to the range of effects identified and the variety of responses of different species, phyla etc. Hence, a translation of results into policy poses several problems for modellers.

14.2 Approaches and methodologies

In contrast to ocean circulation models that rely on the well-established Newton's laws, there are no known fundamental equations that govern marine ecosystems. There is not even consensus on biological invariants that may be used as prognostic variables of a marine ecosystem model. Traditionally, most biogeochemical models and lower-trophic planktonic ecosystem models partition the ecosystem into nutrients, phytoplankton, zooplankton, and non-living particulate and dissolved organic matter, but the more detailed level information on species and the full suite of biological/ecological dynamics needed to address particular questions, such as ocean acidification, cannot always be easily mapped onto this traditional picture. One approach is to make models more complex, for example by adding multiple plankton functional types (PFT models). No model, simple or complex, has yet demonstrated a fully successful reproduction of observed global patterns and temporal variations of biomass or of biogeochemical tracers such as nutrients, carbon, oxygen and total alkalinity within the observational uncertainty. This does not only reflect the yet oversimplified description of biological drivers, but is also attributed to the representation of ocean physics.

It is noteworthy that increased complexity comes at the cost of having to constrain more model parameters (e.g. growth rates, mortality rates, grazing rates), about which we have only very limited information. Moreover, the spread of the biogeochemical function "calcification" across auto- and heterotrophic organisms, as well as the variety of species-specific responses to acidification found in calcifying species (e.g. Fabry, 2008), makes a generic PFT type parameterisation problematic. A further complication is that it is unclear how such models (as well as simpler models) could adequately describe adaptation to environmental changes. Promising new modelling approaches include trait-based models in aquatic ecology. These new models let the ecosystem self-assemble from a large number of species, and biodiversity, and to some extent adaptation, can be emergent features of such models (Norberg *et al.*, 2001; Bruggeman & Kooijman, 2007; Follows *et al.*, 2007). An exhaustive quantitative comparison against field observations has not been done for such models. While these approaches raise additional parameterisation problems in terms of the rule choices for the energetic and metabolic trade-offs, the number of parameters to be set by the person running the model is expected to be smaller than for multiple PFT models.

So far, there are broadly two types of modelling approaches. In the first approach, one attempts to build models based on mechanistic principles, i.e. some reasonably correct representation of physiological and biogeochemical processes that describe the exchange of matter and energy among the different compartments of an ecosystem model. In the other approach, one uses empirical relationships derived from culture, mesocosm or observational studies, and sometimes results from statistical regressions of simple functional relationships against measurements. A subset of the latter, empirical, category include remote sensing algorithms, that contribute valuable information on biological variability (e.g. productivity, calcifier biomass and biomineralisation rates) and when combined with physical data may be useful for interpolating surface water chemistry in space and time (Gledhill *et al.*, 2008). The former, mechanistic, approach has the disadvantage of requiring possibly many parameters (not all of which can be constrained without becoming empirical again), but there is no *a priori* reason why such models cannot be used in predictive mode, as long as the changing drivers are correctly described and incorporated into the process descriptions. The empirical approach is often unsuitable for making predictions as, in general, the sensitivity of these relationships to environmental change, such as warming or acidification, has not fully been established and can therefore not be properly accounted for by the models. A notable exception is empirical models based on observations that encompass future variability of environmental conditions by either considering past and present natural variability or perturbation experiments.

The seawater carbonate system is, in contrast, well constrained. Equilibrium constants are well known, and although there are variations in particular constants emerging from different studies, a consistent and robust approach is generally possible (e.g. Zeebe & Wolf-Gladrow, 2001; Dickson *et al.*, 2007). Typically models use measured dissolved inorganic carbon concentration and measured or estimated total alkalinity as the master variables from which pH, $p(CO_2)$, concentrations of bicarbonate and carbonate and saturation state of different carbonate minerals are calculated. On ocean basin scales this approach is reasonably robust, and total alkalinity can be derived from salinity according to a number of basin-specific linear relationships. Unfortunately, these relationships are at best approximate in shelf seas, where total alkalinity is influenced by significant biological and riverine signals, coupled with high spatial and temporal heterogeneity (Friis *et al.*, 2003; Thomas *et al.,* 2008). These processes are also susceptible to change (e.g. riverine total alkalinity; Raymond & Cole, 2003) and potential changes must be factored into predictive scenarios. It is recommended that total alkalinity be included in biogeochemical ocean circulation models as prognostic tracer rather than being diagnosed from empirical fits to salinity.

With respect to the production of biogenic particulate inorganic carbon (PIC), which in models is usually associated with calcite (disregarding other carbonate minerals), a large variety of parameterisations have been used. Many models assume that PIC production is proportional to primary production or export production, thereby emphasising the role of the $CaCO_3$ cycle in the Earth system. This is fundamentally different from an attempt to assess impacts on the ecosystem level. These parameterisations are often independent of the carbonate chemistry (e.g. Moore *et al.*, 2002; Schmittner *et al.*, 2008). Some models take into account a control of PIC production by the carbonate chemistry (Heinze, 2004; Gehlen *et al.*, 2007; Ridgwell *et al.*, 2007) though different models use different controls (pH, CO_2, CO_3^{2-}, Ω) and different functional forms (linear, sigmoid, power law) describing either PIC production or the ratio of PIC to POC (particulate organic carbon) production. While some of the variables describing the carbonate system are temperature dependent, some models explicitly or, via primary production, implicitly include a temperature dependence in the parameterisation of the PIC production. Most models either explicitly or implicitly assign $CaCO_3$ production to photosynthetic coccolithophores and do not yet try to capture $CaCO_3$ production by zooplankton (foraminifera, pteropods). An early example considering zooplankton together with a consideration of the difference in mineralogy (pteropod aragonite) is the study of Gangstø *et al.* (2008).

The different parameterisations of PIC production and its sensitivities to changes in temperature and carbonate chemistry can lead to very different results. When applied to a global warming scenario, different models may even predict different signs in the change of PIC production. For example, a business-as-usual emission scenario leads to a (CO_2 driven) reduction of PIC production over the next few hundred years in the model of Heinze (2004), whereas essentially the same scenario leads to a (temperature-driven) increase in PIC production in the model of Schmittner *et al.* (2008). The former model run neglects warming effects and assumes a linear relationship between PIC production and CO_2, the later model assumes no direct impact of the carbonate chemistry on PIC production, but includes a temperature effect. Gangstø *et al.* (2008) include a combination of both global warming and CO_2 effects and predict an overall reduction of PIC production. To the authors' knowledge, model parameterisations have not yet been tested against experimental data sets that yield information about the combined effect of warming and acidification on calcium carbonate production and dissolution. These data sets are currently becoming available and will allow an evaluation of model parameterisations in the near future.

Ocean acidification will also affect the vertical transport and remineralisation of PIC and will thus alter the distributions of total alkalinity and dissolved inorganic carbon. Abiotic carbonate dissolution rates increase non-linearly as saturation states decline below 1. The upward shoaling of the saturation horizon will therefore decrease the depth at which sinking particles begin to dissolve in the water column. Changes in euphotic zone biological populations and community composition also could alter particle size distributions and sinking speeds as could changes in the structure and function of mesopelagic food webs. Presently, many biogeochemical models use relatively simple, non-mechanistic parameterisations for organic and inorganic particle remineralisation such as fixed exponential length scales or power laws that are independent of seawater chemistry.

Other implications of acidification are relevant to element cycling and ecological questions. Phytoplankton functional groups have varying sensitivities to CO_2 availability (Tortell *et al.*, 2002, 2008; Rost *et al.*, 2003), with studies showing a shift away from calcifiers to diatoms at low pH and elevated CO_2. Nutrient speciation, nitrification (Huesemann *et al.*, 2002) and nitrogen fixation (Hutchins *et al.*, 2007; Levitan *et al.*, 2007) are all sensitive to pH and/or CO_2. Nutrient uptake stoichiometry may be affected by changes in community composition and vice versa. Phytoplankton uptake and export C:N ratios have also been shown to be CO_2 sensitive (Riebesell *et al.*, 2007). These processes are generally not included in present generation models, apart from specific sensitivity studies (e.g. Oschlies *et al.*, 2008).

A much wider range of models may need to be involved for fully assessing the biological impacts of ocean acidification. These could include high-resolution regional models applied to questions on open ocean eddies, coastal dynamics or coral reefs. Models of higher trophic levels will be required with more detailed life histories of specific organisms (e.g. larvae of molluscs, crustaceans, finfish). Higher trophic levels are often treated via individual-based models that track individual organisms (or groups of organisms), compute biological interactions and responses as a function of time and space along the Lagrangian particle trajectory, and incorporate behaviour (e.g., vertical migration, swarming). Other useful types of models are those oriented towards marine resource management (fisheries) and conservation (e.g. corals, biodiversity), and models of socio-economic processes and ecosystem services.

14.3 Strengths and weaknesses

A strength of numerical models is their purely mathematical description. In principle, the clarity of this “language” should leave no room for ambiguities. However, modern numerical models have become more and more complex, culminating in several tens to hundreds of thousands lines of code for current coupled carbon-climate models. One issue is code errors, the bane of existence for numerical models. Another issue is the coupling of distinct processes required for studying system dynamics. As a result, the behaviour of any particular parameterisation in a model is sensitive to the behaviour of many other parameterisations, often in ways that are non-intuitive until the actual coupling is conducted. A normal user of such models will not be able to carefully read through and understand the entire code, and careful checks are needed to establish with confidence that newly added model components work correctly when combined with the rest of the code. Biogeochemical tracers are, for example, not only affected by the biotic source or sink terms. They are also affected by physical transport processes such as advection, diapycnal mixing, isopycnal mixing, sometimes air-sea exchange, dilution by rain or river run-off, or sinking of particles. Although exact equations for fluid motion are available (the Navier-Stokes equations), one cannot resolve all of the important time and space scales and therefore needs to rely on subgrid-scale parameterisations for processes such as mixing and air-sea exchange. All these processes are commonly dealt with in different subroutines at different locations of the complex code. A common model user will, in general, not want to or not be able to go into the details of all these code parts. This is general scientific practice (not many experimentalists will know everything about the components of their measurement devices), but any flaws in the code parts or in the way they are combined may significantly affect the simulated biogeochemical tracer distributions. Apart from mass conservation, no generally accepted biogeochemical model tests are available, and the appropriate model setup will depend on the experience and prudence of the individual modeller.

Acidification is not the only factor with implications for the marine system, and processes sensitive to ocean acidification are likely to be affected also by climate change (changes in temperature, surface fluxes, transport, light, mixing and species interactions) and direct anthropogenic drivers such as fishing and eutrophication. This complexity underlines the utility of a modelling approach that has the potential to address multiple drivers, particularly as the strongly non-linear interaction of these vectors and the non equilibrium state of marine ecosystems make empirical/statistical based predictions questionable. For example, physical processes sensitive to climate change induce variability in the carbonate system (i.e. latitudinally, Orr *et al.* (2005) or due to upwelling, Feely *et al.* (2008)). Altered regional rainfall patterns which, along side changes in land use and industrial processes, will modify fluvial inputs to coastal systems affecting nutrients, optical properties, dissolved inorganic carbon and total alkalinity (Raymond & Cole, 2003; Gypens *et al.*, 2009). Species and communities are likely to shift their geographic ranges as temperatures increase (e.g. Beaugrand *et al.*, 2002), introducing different phenologies, acidification sensitivities and trophic transfer potential. There are also processes and systems directly affected by both temperature and acidification. Coral calcification is vulnerable to both thermal stress from climate change and lowering saturation states driven by acidification (e.g. Reynaud *et al.*, 2003) and sensitivity to nutrient concentrations has also been identified (Langdon & Atkinson, 2005). There is also clear evidence that combined CO_2 and temperature stress induces amplified effects on higher trophic level organisms (Pörtner *et al.*, 2005; Pörtner & Knust, 2007; Pörtner & Farrell, 2008).

14.4 Potential pitfalls

Numerical models are written in computer languages that must be translated by machine-specific compilers into machine-readable commands. As a matter of fact, the same model may yield different results when run on different computers or even on different CPUs (central processing units) of the same computer. Usually, these differences are small, for example rounding errors at the last digit. For properly written codes this should not significantly affect the results of the simulation. Another issue are compilers, themselves computer codes with possible errors, that have different "risk options" with higher risks often being very attractive as they lead to faster performance of the code. Model results obtained under different "risk options" are often different. It is generally hoped, but rarely shown, that these differences do not significantly affect the model results.

A second issue arises when converting model equations from the continuous or analytical form into discretised form and then solving those discretised equations using numerical methods. Some care has to be taken to ascertain that the solution algorithm (e.g. Euler, Runge-Kutta, etc.), in combination with the choice of time and space discretisation schemes, does not lead to unacceptably large numerical errors. Many climate models have built-in checks for some stability criteria for the simulation of fluid flow, but biogeochemical and ecological model components often resort to pragmatic algorithms (for example, Euler forward in time, clipping of spurious negative tracer concentrations). It is hoped and expected that such issues are of minor importance for the model solution, but this is rarely shown nor is it evident for the often highly nonlinear systems.

Numerical tracer advection schemes are required for all models with spatial dimensions, and these numerical approximations can introduce artificial extrema or, alternatively, overly smooth simulated tracer fields. The choice of advection scheme can have substantial impacts on chemical and biological tracers, particularly in regions with sharp spatial gradients. This can be especially troublesome near the surface where numerical errors can lead to unphysical, negative tracer values. While no advection scheme can fully meet all desired metrics, new higher-order methods are available that provide decent compromises at reasonable computational cost.

Conceptual pitfalls are that we very likely miss some key physiological effects at the organism level in our models. For example, mechanistic descriptions of biogenic calcification or of the sensitivities of different zooplankton life stages or fish larvae to changes in carbonate chemistry are not yet available. Furthermore, food web dynamics is not understood well enough to propagate impacts on one trophic level or specific taxonomic groups (say pteropods or cold-water corals) to higher trophic levels and the whole ecosystem.

14.5 Suggestions for improvements

It is vital that the entire model code used in publications is archived and available so that experiments can be repeated. Many journals now explicitly allow for electronic supplementary material; others like the new open access journal Geoscientific Model Development encourage publication of model descriptions. A minimum requirement should be the publication of the mathematical equations used in the respective model. From a biogeochemist's viewpoint this should be the biogeochemical source and sink terms of any coupled carbon-climate model. However, it should be kept in mind that apparent details such as the algorithms used to transport tracers may turn out to be significant for the model results, as are the initial conditions, forcing data and computational details. Similar to laboratory logbooks used in experimental work, it is good practice, and recommended here, to archive the entire source code, make files, compiler options, operating system and machine version used to obtain the published results. Testing of models or model components by others in the form of collaborative projects is encouraged, as this promotes two-way knowledge exchange.

Evaluation of models is a pre-requisite for establishing (un)certainty and model utility. Far too little attention has historically been paid to evaluation (Arhonditsis & Brett, 2004) and many publications still do not consider model correctness with any acceptable detail. One particular practice is to rely solely on visual comparisons, which have no quantitative basis. Formal evaluation metrics are readily available (Doney *et al.*, 2009; Stow *et al.*, 2009) and these provide an ability to gauge model improvements and to identify process, spatial or temporal problems with model construct. Other multivariate techniques (e.g. Allen & Somerfield, 2009) provide an ability to test the emergent properties of a model, for example whether the relationships between key variables in the model replicate those in the observations. This approach can be useful in dynamic systems where the model setup is rarely able to exactly mimic events in space or time because of, say, a lack of accuracy in underlying physical models or boundary conditions, but the essential dynamics of the ecosystem model is potentially reasonable.

Evaluation can take many forms. Where observations are sparse, an evaluation of process descriptions is useful. In particular, forecast scenarios that clearly cannot be evaluated *per se,* can be evaluated in a hindcast simulation. Evaluation can also be addressed as a stand-alone publication, which allows sufficiently detailed treatment, especially for complex model systems (e.g. Holt *et al.*, 2005; Lewis *et al.*, 2006; Allen *et al.*, 2007).

Despite driver uncertainties in marginal seas, the carbonate system is well constrained. Therefore an absolute requirement for models is the correct treatment of the carbonate system. Standard CO_2 system model code is publically available through the Ocean Carbon-Cycle Model Intercomparison Project (OCMIP) web site (http://www.ipsl.jussieu.fr/OCMIP/). The user should refer to the most recent developments.

A concern is the obvious lack of biological detail in global or earth system models and the less obvious identification of the level of model complexity needed to answer the respective scientific question. Whilst complexity is often limited by computational systems and important feedback mechanisms are likely to be omitted, more complex models tend to be much more difficult to understand and to calibrate. There is a case for stronger iteration with regional, ecologically complex models that may be better constrained by the available data sets than global models and that may help to identify important processes that could be tested in global simulations. In particular, variable stoichiometry (carbon to nutrients, carbon to chlorophyll) is being identified as an important quality of marine ecosystem models.

The use of model results for policymaking requires some care. For example, the highly variable predictions of warming from climate models initially created uncertainty in public and policy response, which may have undermined the speed with which climate change became globally recognised. In this respect, the IPCC approach to use a probabilistic reporting envelope is highly valuable (despite inherent problems of such a probabilistic description; Betz, 2007), as are the coherent scientific summaries from the "Oceans in a High CO_2 World" symposiums for example. Still, understanding uncertainty and rigorous evaluations are vital components for robust science. This specifically holds for the use of models. Although each model simulation is usually deterministic, i.e., it will report a unique answer for a given scenario, uncertainty comes into play via initial and boundary conditions (in particular the considerable uncertainty in future CO_2 emissions), via our incomplete knowledge of the governing natural laws, and via uncertainty in the parameter values that are used in the model equations. In addition, ensemble approaches, which explore say parameter or driver uncertainty and deliver a probabilistic conclusion, are valuable as are model–model intercomparison exercises that explore apparent disagreements in results.

14.6 Data reporting

The archiving of model output has to follow the general rules outlined with respect to data and metadata reporting and archiving outlined in chapter 15. Similar to protocols used in experimental work, it is therefore good practice to archive the entire code, make files, and compiler options used to obtain the published results.

14.7 Recommendations for standards and guidelines

1. Report all equations, parameterisations and parameter values used in publications
2. Model code must be archived, ideally under version control. If possible, it should be made publicly available.
3. Carbonate chemistry must be correctly calculated (the most recent OCMIP protocol is recommended: http://www.ipsl.jussieu.fr/OCMIP/)
4. Models must be evaluated against observations and their uncertainty documented and accounted for when drawing conclusions.
5. Ongoing data compilation and synthesis efforts are needed for model evaluation; they must be pursued and amplified. For example, data sets of seasonal changes and secular trends in carbonate chemistry, distribution and rate of calcification and biological responses to seawater chemistry are very useful. A good example is the EPOCA/EUR-OCEANS data compilation project (http://www.epoca-project.eu/index.php/What-do-we-do/Science/Data.html).
6. New targeted laboratory mesocosms and field perturbation experiments should be conducted to test and improve the functional form and parameters for parameterising biological processes.

14.8 References

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