

Evaluation of the Current State of Mechanistic Aquatic Biogeochemical Modeling: Citation Analysis and Future Perspectives

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We examined the factors that determine the citations of 153 mechanistic aquatic biogeochemical modeling papers published from 1990 to 2002. Our analysis provides overwhelming evidence that ocean modeling is a dynamic area of the current modeling practice. Models developed to gain insight into the ocean carbon cycle/marine biogeochemistry are most highly cited, the produced knowledge is exported to other cognitive disciplines, and oceanic modelers are less reluctant to embrace technical advances (e.g., assimilation schemes) and more critically increase model complexity. Contrary to our predictions, model application for environmental management issues on a local scale seems to have languished; the pertinent papers comprise a smaller portion of the published modeling literature and receive lower citations. Given the critical planning information that these models aim to provide, we hypothesize that the latter finding probably stems from conceptual weaknesses, methodological omissions, and an evident lack of haste from modelers to adopt new ideas in their repertoire when addressing environmental management issues. We also highlight the lack of significant association between citation frequency and model complexity, model performance, implementation of conventional methodological steps during model development (e.g., validation, sensitivity analysis), number of authors, and country of affiliation. While these results cast doubt on the rationale of the current modeling practice, the fact that the Fasham et al. (1990) paper has received over 400 citations probably dictates what should be done from the modeling community to meet the practical need for attractive and powerful modeling tools.

Introduction

Mechanistic biogeochemical models have had a central role in aquatic ecosystem research, e.g., they have been used for elucidating ecological patterns or aspects of system dynamics that are technologically or economically unattainable by other means (1, 2); they have formed the scientific basis for

environmental management decisions by providing a predictive link between management actions and ecosystem response (3, 4); they have provided an important tool for understanding the interactions between climate variability and plankton communities, and thus address questions regarding the pace and impacts of climate change (5, 6). Their role as a key research tool for understanding and quantitatively describing aquatic ecosystems can also be indicated by recent review/synthesis papers that assessed their methodological consistency and performance (7), underscored the importance of effectively coupling physical and biogeochemical models (8, 9), and identified the major problems, technical or conceptual advances and future perspectives (10–12).

Despite the significance and considerable attention, a recent evaluation of the current state of mechanistic aquatic biogeochemical modeling across the range of temporal and spatial scales typically utilized has provided controversial quantitative and qualitative information (7). Specifically, one of the major findings was that the performance of existing mechanistic aquatic biogeochemical models declines as we move from physical–chemical to biological components of planktonic systems and that the consideration of longer simulation periods and increased model complexity has not improved model performance. The same analysis also indicated that there was considerable methodological inconsistency regarding the steps followed during the development stages of the models; i.e., conventional modeling procedures, such as sensitivity analysis, validation, or even assessment of goodness-of-fit were not applied in a high proportion of the published modeling studies (7; see their Figure 2). Given the convincing presentation in several classic modeling textbooks of what “rational model development” is (13, 14), the absence of a systematic methodological protocol widely followed from the modelers was surprising.

The objective of this study is to present a second quantitative assessment of the current state of aquatic biogeochemical modeling by focusing on their citation frequency and identifying the factors that determine the citation rates. Our aim is to analyze how has the modeling community received and applied the 153 models published from 1990 to 2002. Thus, this study will allow us to gain insight into what characteristics of a model are more attractive to the potential “consumers” and may influence the frequency of its use and subsequent citation. First, we compiled the demographic profiles of the papers that cited the 153 modeling studies (authors, journal, publication year, institution, scientific discipline, and country of affiliation) and

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identified the basic features of the “market”/potential users of mechanistic aquatic biogeochemical models. Then, we examined the factors that determine the citation frequency of the modeling papers; we tested the association between citation rates and characteristics of the published modeling studies: type of the ecosystem modeled, journal impact factor, authorship characteristics, methodological consistency, and model performance. Our main question is to determine whether the social factors, the quality of the modeling study, or the questions being addressed is the basic criterion for the recognition that a modeling study receives. We conclude our presentation with a critical discussion of some of the outstanding challenges of the current and future modeling practice.

Citation Rates of Mechanistic Aquatic Biogeochemical Modeling Papers

Our citation analysis builds upon the results of an earlier study focused on the ability of biogeochemical models to predict spatial and temporal patterns in the physical, chemical, and biological dynamics of planktonic systems (7). As noted there, the literature was searched using (i) the electronic databases “Aquatic Sciences & Fisheries Abstracts”, “BIOSIS previews”, “ISI Web of Science”, and “ScienceDirect”; and (ii) the keywords “eutrophication model(l)-ing”, “NPZ model(l)-ing”, “water quality model(l)-ing”, “phytoplankton model(l)-ing”, “freshwater model(l)-ing”, “ocean model(l)-ing”, and “biogeochemical model(l)-ing”. To be included in the analysis, studies had to present graphs or tables in which observed data were compared to model outputs; 153 papers fit this criterion (7; see Appendix 1). These same 153 papers are analyzed here for their citation records. Papers that modeled the aquatic fate and transport of individual contaminants or groups of contaminants, without specific reference to nutrient cycles and plankton dynamics, were not included. Nor were studies that provided only qualitative (conceptual) modeling and/or sampling results. We searched the electronic database Web of Science (<http://www.isiwebofknowledge.com/index.html>) to extract quantitative information (journal, institution and country of affiliation, scientific discipline, and publication year) pertinent to the papers that cited the 153 mechanistic aquatic biogeochemical modeling studies. The papers used in the original meta-analysis were published in 34 journals and, not surprisingly, the large majority of both cited and citing articles originated from journals that place emphasis on ecological modeling (e.g., *Ecological Modeling*, *Journal of Marine Systems*, and *Deep Sea Research*; see Figure 1). The modeling studies considered in our analysis received citations from papers published in 246 different journals that spanned a wide range of disciplines. The latter finding is probably an indication that mechanistic aquatic biogeochemical modeling produces “exportable” knowledge of wider scientific interest. The 153 modeling studies were cited 21 times on average, while the median value and the interquartile range (difference between the 75th and the 25th percentile) of their citations were 13 and 18, respectively.

Among the modeling papers published during the study period (1990–2002), the Fasham et al. (15) food web model stands out as the most cited paper in the process-based aquatic biogeochemical modeling literature (Table 1). Interestingly, more than half (53.09%) of this paper’s 405 citations were received within the last 5 years, which indicates that several aspects of this study (e.g., novel model formulations, ecological structure, sensitivity analysis, ecosystem studied) are still appealing to contemporary research. For example, the Fasham et al. (15) study was the first modern model to explicitly consider separate formulations for nitrate and ammonium flows that symbolize new and regenerated production (i.e., the Eppley-Peterson f-ratio paradigm),

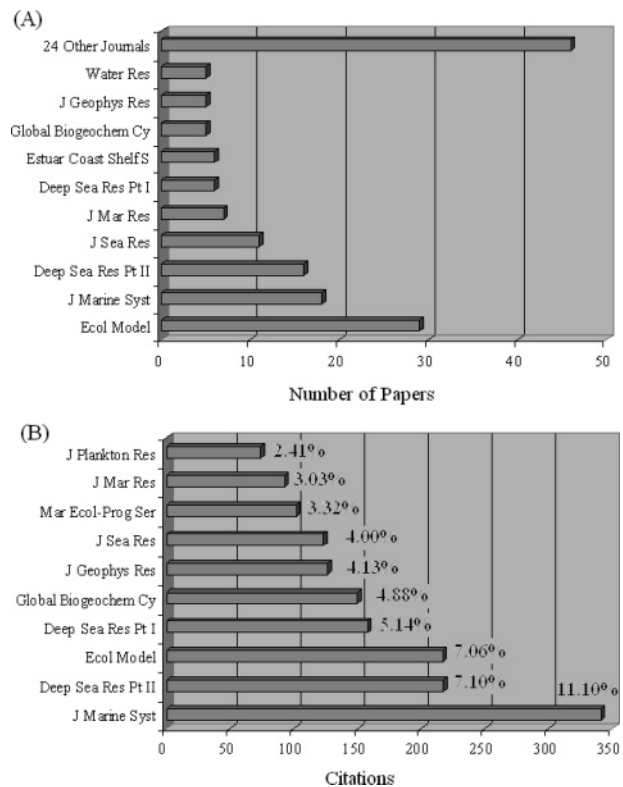


FIGURE 1. Frequency histogram of the journals that (a) publish and (b) cite mechanistic aquatic biogeochemical modeling papers. Citations from the paper Arhonditsis and Brett (2004) were subtracted from the journal *Marine Ecology-Progress Series*.

respectively. In addition, the same model was also created to give outputs directly compatible with flow analysis routines (16) and was the first to be coupled to a basin-scale circulation model (17). The late 1980s and early 1990s were a time when a couple of pioneers in the ocean biogeochemistry community had started to incorporate biogeochemical processes into ocean general circulation models. The Fasham et al. (15) model was simple enough to be implemented in ocean general circulation models or variations of it in a wide range of other applications (17, 18). In this respect, the Fasham et al. (15) study came up with the right idea at the right time; a phenomenon that is often seen when a major breakthrough starts a new field.

Another ocean modeling study by Doney et al. (19) was the second most highly cited paper (107 citations). In this study, the authors introduced a simple four-compartment (nitrogen–phytoplankton–zooplankton–detritus) biological model with an interesting parameterization (e.g., photoadaptation, variable chlorophyll-to-nitrogen ratios) along with a physical mixed-layer model that improved the simulation of the plankton dynamics in the oceanic euphotic zone. Several other simple ecological models with aggregated plankton state variables and 3-dimensional (20, 21) or simpler spatial structure (22, 23) can be found in the top ten of the most highly cited modeling papers. However, there are also complex modeling approaches (ERSEM, SWAMCO) with multiple biogeochemical cycles and several functional plankton groups considered that have received considerable attention (24–26). Generally, nine ocean modeling studies were included in the list of the ten most highly cited papers, with the only exception being the paper by Cerco and Cole (27). The latter paper presented the application of the three-dimensional CE-QUAL-ICM model to the Chesapeake Bay, and the main objective was to assist eutrophication management.

TABLE 1. Ten Most Highly Cited Papers in the Field of Mechanistic Aquatic Biogeochemical Modeling (Study Period 1990–2002)

authors	year	journal	ecosystem	complexity	citations ^a
Fasham et al.	1990	<i>J. Mar. Res.</i>	Atlantic Ocean	simple	405
Doney et al.	1996	<i>Deep-Sea Res. Part II</i>	Atlantic Ocean	simple	107
Fasham et al.	1993	<i>Global Biogeochem. Cycles</i>	Atlantic Ocean	simple	84
Six and Maier-Reimer	1996	<i>Global Biogeochem. Cycles</i>	Pacific Ocean	simple	81
Cerco and Cole	1993	<i>J. Environ. Eng. ASC.</i>	Chesapeake Bay	complex	55
Lancelot et al.	2000	<i>Deep-Sea Res. Part I</i>	Atlantic Ocean	complex	55
Sharples and Tett	1994	<i>J. Mar. Syst.</i>	North Sea	simple	51
Aksnes et al.	1995	<i>Ophelia</i>	North Sea	simple	46
Broekhuizen et al.	1995	<i>J. Sea Res.</i>	North Sea	complex	46
Ebenhoh et al.	1995	<i>J. Sea Res.</i>	North Sea	complex	46

^a Reported date: 18 November 2005 (ISI Web of Science).

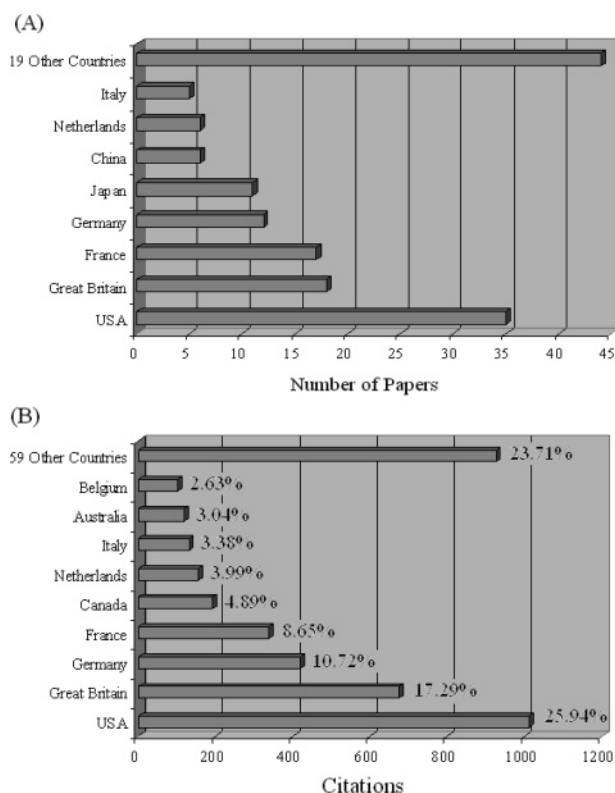


FIGURE 2. Country of affiliation of the authors who (a) published (reprint author) and (b) cited mechanistic aquatic biogeochemical modeling papers.

Based on the reprint author's country of affiliation, we infer that a total of 27 countries contributed to the published modeling literature during the period 1990–2002 and that nearly half (45.5%) of these studies were originated from U.S., British, and French institutions (Figure 2a). Likewise, the same countries (along with Germany) represent 62.6% of the citations received, although researchers from 68 different countries participated in the authorship of the citing articles (Figure 2b). These trends clearly show that the field of mechanistic aquatic biogeochemical modeling is dominated by a relatively small group of countries that account for the large majority of the cited and citing articles. Furthermore, the United States shows a comparative advantage over the European countries in terms of the frequency of producing models and consuming the generated knowledge (Figure 2). Nonetheless, a closer look on the ten institutions (Table 2) that mostly cite mechanistic aquatic biogeochemical modeling papers indicates that only two were from the United States (Woods Hole Oceanography Institute and University of Washington), whereas the Plymouth Marine Lab (Great Britain) and the University of Hamburg (Germany)

TABLE 2. Ten Institutions That Mostly Cite Mechanistic Aquatic Biogeochemical Modeling Papers

name	country	citations ^a
Plymouth Marine Lab	Great Britain	229
University of Hamburg	Germany	133
Woods Hole Oceanography Institute	United States	121
University of Kiel	Germany	97
Southampton Oceanography Centre	Great Britain	94
University Paris 06	France	92
Bidston Observatory	Great Britain	92
Alfred Wegener Institute	Germany	85
Centre National de la Recherche Scientifique	France	73
University of Washington	United States	68 ^b

^a Reported date: 18 November 2005 (ISI Web of Science). ^b Citations from the paper Arhonditis and Brett (2004) were subtracted from both the University of Washington and Duke University.

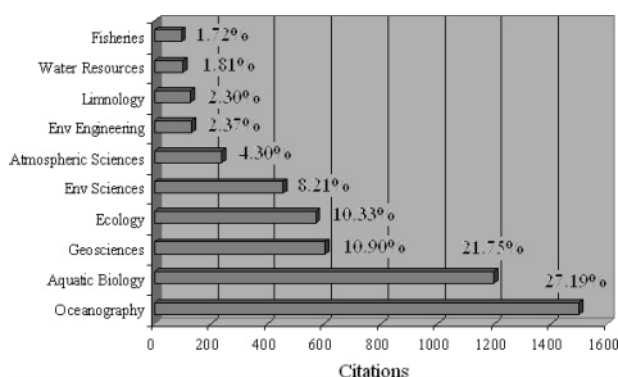


FIGURE 3. Frequency histogram of the scientific classification (subject category) of the papers that cite mechanistic aquatic biogeochemical modeling papers.

were the top-ranked institutions regarding the number of publications that cite modeling studies.

The citing articles were classified in 60 different disciplines. Several of these disciplines (e.g., astronomy, computer science, software engineering, plant sciences, genetics, and heredity) had no apparent association with mechanistic aquatic biogeochemical modeling, which is probably another indication that this field produces scientific knowledge (e.g., methodological advancements for system analysis, ecological questions addressed) that can have broader application and assist quite different subject areas. Oceanography is the most popular subject category of the articles that cite mechanistic aquatic biogeochemical models and more than 27% (approximately 1500 counts) of the total citations were related to this research topic (Figure 3). The second most popular thematic area was marine and freshwater biology (21.75%) followed by geosciences (10.90%) and ecology (10.33%). Interestingly, disciplines more closely associated with en-

vironmental management, e.g., environmental sciences (8.21%), environmental engineering (2.37%), and water resources (1.81%), account for a relatively low proportion of the total citations received.

Citation Rates and Individual Study Characteristics

We examined the association between citation rates and several characteristics of the published modeling studies: type of the ecosystem modeled, journal impact factor, authorship characteristics, methodological consistency, and model performance. The immediacy index (i.e., the average number of times that an article published in a specific year within a specific journal is cited over the course of that same year <0.500) and cited half-life (i.e., the number of years, going back from the current year, that account for 50% of the total citations received by the cited journal in the current year >5 years) values of the journals that publish modeling studies raised questions related to the effects of publication year differences on the statistical analysis results. While we recognize that the citation patterns of the more recently published modeling studies are not completely revealed by our analysis, we found that the standardization of the citation rates by the publication year (i.e., partial correlation and analysis of covariance) did not alter the inference regarding the statistical significance of the following results.

Using as a criterion the type of the ecosystem modeled, the published modeling studies were classified in six categories, i.e., “Coastal area-Estuary”, “Mesocosm”, “Bay-Lagoon-Harbor”, “Lake-Reservoir”, “Ocean-Sea”, and “River”. Ocean modeling studies have received significantly higher citations ($F = 7.87$, $df = 5$, $p < 0.001$) among the various ecosystem types (Figure 4a). [Note that the three—out of five—most highly cited papers in the category “Mesocosm” were preliminary model examinations in experimental set-ups prior to the actual application to oceanic systems]. Furthermore, the higher citation frequency of ocean modeling studies can also explain the significantly higher citations of papers ($F = 8.65$, $df = 10$, $p < 0.001$; journals with <5 papers were not considered) published in journals pertinent to the topics of oceanography and/or global climate change. In contrast with a recent study by Leimu and Koricheva (28), we found that paper citation rates were not significantly correlated with the journal impact factor. Interestingly, papers published in specialized modeling journals (e.g., *Ecological Modeling*, *Environmental Modeling & Software*) or prestigious journals in water quality research (e.g., *Water Research*) received fairly low citations. Given the local character of the majority of these modeling studies, the latter finding probably indicates a lack of wider interest in models developed for addressing site-specific environmental management problems or understanding ecological patterns that are not related to ocean dynamics. We also tested whether citation rates of modeling papers differ depending on the reprint author’s country of affiliation. We found that papers by authors from Great Britain, the United States, Germany, and France receive significantly higher citations than authors from other countries ($F = 2.92$, $df = 7$, $p = 0.008$). In addition, we examined the influence of the number of authors and the article length on the citation rates; we found that neither of these factors is associated with the number of citations that the study receives.

Regarding the model complexity role (expressed as the number of state variables) as a model feature that attracts citations, we found that the citation rates of the individual articles were not significantly correlated with the corresponding model complexity ($r = 0.111$, $p = 0.183$). The positive correlation value between model complexity and citations probably reflects an increasing citation trend for models with over 40 state variables (see the respective median value in Figure 5a), although the majority of the highly cited

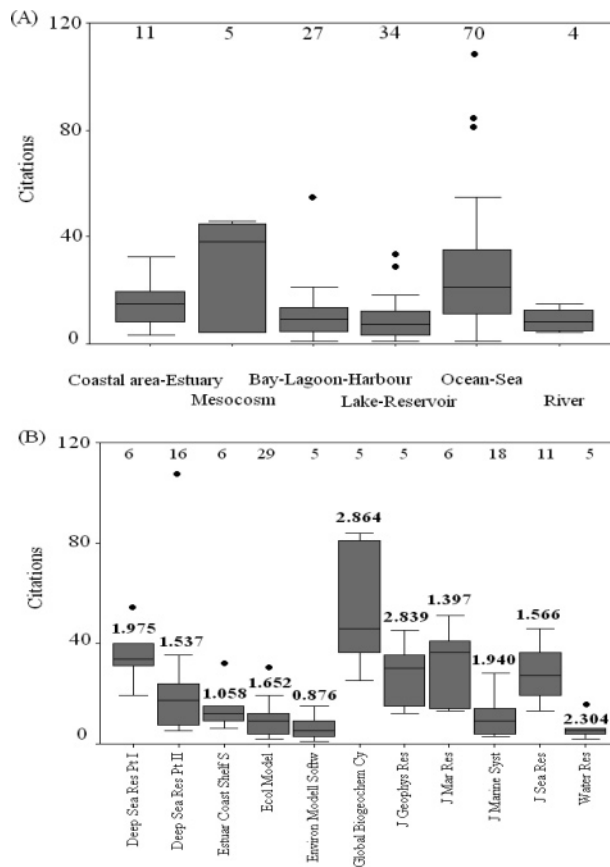


FIGURE 4. Citation frequency for (a) different types of modeled ecosystem, and (b) publishing journals. The journal impact factors are reported above the box-plots. Note that the study by Fasham et al. (1990) is not included in the plot to facilitate the visualization of the inter-group comparisons. [Numbers of studies for each group case are indicated at the top of the two plots].

modeling papers represented simple models with fewer than 10 state variables (Table 1 and outliers in Figure 5a). We also examined whether the methodological consistency of the published modeling studies is a factor that influences their citation rates. The expression “methodological consistency” refers to the extent that methodological steps typically recommended by classic modeling textbooks were actually implemented during model development (i.e., sensitivity analysis, quantification of goodness-of-fit, and validation). Based on the Arhonditsis and Brett (7) classification scheme (see their Figure 2), we found that the citation counts did not differ significantly among studies that conducted (thorough/partial) sensitivity analysis and those that did not ($F = 1.16$, $df = 2$, $p = 0.316$). The citation patterns of the modeling studies were not affected by whether or not the modelers reported assessment of the goodness-of-fit in the original study ($F = 0.05$, $df = 1$, $p = 0.943$; Figure 5b), or by whether or not the model was structurally or predictively validated ($F = 2.03$, $df = 1$, $p = 0.156$). Finally, the authors did not consider model performance as a criterion for citing modeling papers; e.g., citation rates and model performance for the “key” state variable phytoplankton were not significantly correlated ($r = 0.163$, $p = 0.07$; Figure 5c).

What Can we Learn from this Citation Analysis?

Citation frequency and impact factors are increasingly recognized as convenient tools for assessing the importance and utility of scientific research; ideally, high-quality papers should motivate future research and should be used as source of information by subsequent studies in the field (29). In

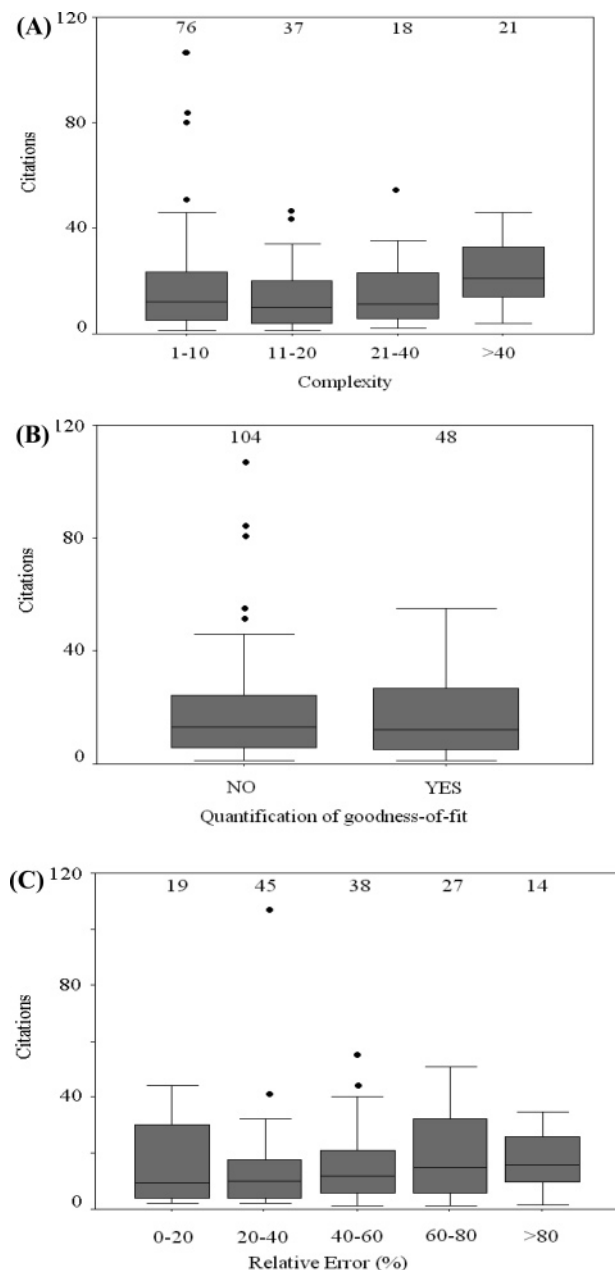


FIGURE 5. Citation frequency for different levels of (a) model complexity (number of state variables), (b) reported assessment of the goodness-of-fit in the original modeling study, and (c) model performance for phytoplankton. Note that the study by Fasham et al. (1990) is not included in the plot to facilitate the visualization of the inter-group comparisons. [Numbers of studies for each group case are indicated at the top of the two plots].

practice, however, there are critical voices that cast doubt on the objectivity of the citation scores and also highlight the role of several subjective (e.g., interpersonal connections, flattery) and social (e.g., nationality, gender, institution) factors that are unrelated with the scientific process (28, 30). Our study examined the effects of some of these commonly reported mis-citation errors and biases vis-à-vis the quality features of the 153 modeling studies considered in the original meta-analysis (e.g., consistency with methodological protocols, model complexity, and goodness-of-fit). We recognize that our results do not reflect the entire spectrum of studies/projects pertinent to aquatic biogeochemical modeling during the study period; there are also other means for communicating scientific research (e.g., books, technical reports, websites) that were not accounted for in our analysis.

Nonetheless, a comprehensive sample from the peer-reviewed literature that covers more than a decade of modeling practice can sufficiently unveil trends, preferences, and biases of the cited and citing articles.

Like other disciplines (31), a small number of countries (e.g., the United States, Great Britain, France, Germany) head the list of nations in the number of publications and citations in the field of process-based aquatic biogeochemical modeling. Model citations are determined neither by the reported performance, model complexity, and methodological consistency nor by the journal published, article length, and number of authors. The type of the ecosystem being modeled was proven to be the most influential factor that shapes the citation patterns of the aquatic biogeochemical modeling papers. Specifically, ocean modeling studies have received considerable attention and overwhelmingly dominate the total citation counts. By interpreting our results, someone can infer that as long as a modeling study addresses aspects of oceanic dynamics is likely to receive more attention, regardless of the features of the model used, methodological protocol followed, and goodness-of-fit obtained. Is this statement valid? Which are the actual factors hidden behind these citation patterns?

Marine biogeochemical numerical modeling has been an indispensable tool for addressing several pressing environmental issues, with the most profound being the understanding of the oceanic response to climate change and illumination of the interplay between plankton dynamics and atmospheric CO₂ levels via several feedback mechanisms, e.g., “biological pump”, calcification (5, 12). Oceans have a major role in the global carbon cycle and their biota have a tremendous socioeconomic value (32). Therefore, the oceanic numerical models offer insights that are appealing to a broader audience and stimulate research that spans a wide range of tightly intertwined disciplines (6). Methodologically, the evolution of the oceanic models has been fairly rational and congruent with the technological constraints and data availability. The majority of the models belong in the family of the Fasham et al. (15) food-web model and consist of a small number of state variables that mainly comprise the limiting nutrient (nitrogen) and highly aggregated biotic compartments (e.g., phytoplankton, bacteria, zooplankton). This class of models has provided simulations of bulk properties, (e.g., timing and magnitude of phytoplankton blooms, primary productivity, nutrient fields) that are usually supported by the existing data (7, 12), while their fairly simple parameterization can overcome major problems of identifiability and has enabled the coupling with general circulation models (21, 33). Thus, their flexible structure, efficiency and ease of understanding have led to an “informal consensus” of their use and can explain the impressively high number of citations that some of these studies have received (Table 1). Furthermore, oceanic modelers are also keener to embrace technical advances to control prediction error or ameliorate problems of underdetermination, e.g., assimilation schemes (5), and more prudent to formulate complex models, e.g., test new ecological theories, include specific plankton functional types, and multiple element cycles (12, 34). Overall, oceanic modeling appears to be a more methodologically coherent and vibrant area of research; the modelers seem to have a clearer picture of what needs to be done to gain scientifically rigorous insights and provide convincing explanations of marine biogeochemical cycles. In this context, the high number of citations and their ability to produce knowledge that is exported to other cognitive disciplines is not surprising.

Contrary to our expectations, model application for addressing environmental management issues on a local scale seems to have languished. The pertinent papers comprise a smaller portion of the published modeling literature; the

number of modeling studies from lakes, reservoirs, coastal embayments, estuaries, and harbors combined was approximately equal to the number of oceanic applications (7; Figure 1b). One plausible reason for the relative underrepresentation of local character studies in the modeling literature might be the inclination of model practitioners to convey their results mainly through technical reports and lack of interest or motivation to publish in the peer-reviewed literature. If this explanation is true, then our analysis is missing some information from site-specific modeling constructs that have been developed for addressing water quality management issues (e.g., eutrophication control).

On the other hand, the majority of the local character modeling studies published from 1990 to 2002 have received fairly low citations; although some of these papers appeared in prestigious journals specialized in modeling or water quality research. Given the critical planning information that these model applications aim to provide, the patterns of esotericism found by our analysis invite further investigation; i.e., why are modeling papers that deal with practical management problems less cited? Apparently, modelers seem to work in isolation and, counter to the interdisciplinary nature of their objectives, show a lack of haste to borrow experiences and new ideas from other disciplines or similar character modeling studies. The greater suite of idiosyncrasies that many streams, lakes, and rivers exhibit may rule out a “methodological consensus”, but does not fully justify the distinctly lower citations received by the majority of these studies. Furthermore, while we recognize that some influential studies in the field of water quality management never appeared in major scientific journals (e.g., 35), the—previously mentioned—limited exposure to the peer-review process is likely to further accentuate the esoteric character of the modeling practice. However, robust modeling tools to address impaired conditions of water bodies are needed now more than ever before; e.g., the costly implementation of total maximum daily loads for pollutants during the next 10–15 years has raised the bar for innovative model developments that can accommodate rigorous error analysis (36). Conceptual weaknesses, methodological omissions, failure to incorporate residual variability, and parameter uncertainty in predictions are more critical when addressing practical management problems (10). In oceanography, the use of models as heuristic tools to elicit conceptual paradigms, to provide semiquantitative (or even qualitative) descriptions and understanding of ecological patterns is still a fundamental objective, while the policy-making process that guides costly management decisions requires predictive tools able to support deterministic statements (and associated errors). Different objectives result in different expectations and standards, which probably explains the different patterns of citation and recognition between the two groups of the modeling community. Yet, modelers are more reluctant to adopt new ideas in their repertoire when addressing environmental management issues; for example, data assimilation techniques (37), formulations that consider new ecological theories (e.g., stoichiometric nutrient recycling theory; 4), and novel calibration methods (38) are relatively rare. In many respects, the practice underlying the water quality modeling—decision making interface has remained unaltered during the last three decades. Failure to engage novelty and creativity with solutions to practical environmental problems has inevitably resulted in unattractive modeling products that cannot export knowledge to other disciplines.

Future Perspectives

We believe that the mechanistic aquatic biogeochemical modeling can benefit from the examination of the reasons that made several ocean modeling papers so successful; namely, these studies introduced breakthrough ideas that

came at a time when the community was ready for them. Viewed from this perspective, a great deal of the research that has occurred over the past 15 years represents incremental learning without the capacity to truly inspire significant new breakthroughs. This is the usual trajectory that most new fields of knowledge follow. However, this view does invite one to ask what it would take to prime the pump for the next Fasham et al. study to come along? Several review/synthesis papers in aquatic ecosystem modeling have provided insights into the current state of the field, and have highlighted the major challenges and future directions of research (2, 5, 9, 10, 34). Development of new model formulations, empirical representations of plankton functional types, emerging techniques of data assimilation and model optimization, effective integration of physics with biology, novel uncertainty analysis techniques, and strategies to improve the contribution of complex models to ecological theories are some of the ongoing and future thrusts in progress. Among the variety of interesting suggestions for model improvement, we will elaborate on two issues that warrant special consideration: i.e., the pressure for increasing model complexity and the need for developing effective tools for model uncertainty assessment.

Despite several sober views in the literature (9, 12), there is an increasing demand for more complex models; for example, there are requirements for explicit treatment of multiple biogeochemical cycles and increase of the functional diversity of biotic communities, e.g., plankton functional types that can carry out key biogeochemical processes (5). There are even propositions for mechanistic description of processes that produce random (or quasi-random) events (39). Generally, the premise for constructing complex models is to mirror the complexity of natural systems and account for ecological processes that can become important in future hypothesized states, and thus increase their predictive ability (40). In essence, modelers believe that if they can “get the processes right” in the mathematical equations, then the model truly is a mimic of the real system. However, if we inspect the theory behind process description, we will realize that all models are drastic simplifications of reality that approximate the actual processes (see Supporting Information, Box 1: How feasible is the “correct process description?”), and all parameters are effective (e.g., spatially and temporally averaged processes) values unlikely to be represented by a fixed constant (see Supporting Information, Box 2: What do model parameters represent?). Causal explanations and mechanistic descriptions are scale-dependent and many practical applications are based on simple aggregated summaries. Furthermore, poorly understood ecology, determination of the optimal aggregation level of biotic entities, and understanding the entire suite of direct and interactive effects between system components impose barriers to the potential of success of these reductionistic views on aquatic ecosystem modeling (12). While the increase of the articulation level is certainly an effective means for improving our models, we should not neglect that the increasing complexity also reduces our ability to properly constrain the model parameters from observations, i.e., the number of parameters that must be specified from the data is approximately proportional to the square of the number of compartments (34). In this case, the application of mechanistic models for extrapolative tasks gradually becomes “an exercise in prophecy” rather than scientific action based on robust prognostic tools (41). Our current experience indicates that the forecasting of ecosystem behavior is extremely difficult and even in well-studied, data-rich systems using very sophisticated models, accurate predictions were not feasible (3, 42). Ecosystem dynamics are driven by foreseeable environmental processes which are often confounded with self-organized, complex adaptive behaviors

that are difficult to be predicted (3). Differentiating the predictable from the unpredictable patterns and increasing model complexity accordingly requires careful consideration and should be tightly coupled with critical evaluation of the model outputs; the latter concern underscores the central role of uncertainty analysis.

The importance of investigating the effects of uncertainty on model predictions has been extensively highlighted in the modeling literature (12, 41, 43). Nonetheless, most aquatic mechanistic biogeochemical models published over the past decade did not fully assess prediction error; thorough quantification of model sensitivity to parameters, forcing functions and state variable submodels was only reported in 27.5% of the studies, while 52.9% of the published models were not predictively or structurally validated (7). Regardless if this factor determines (or not) the citations of a modeling study, modelers should understand the necessity for explicitly reporting the uncertainty contributed by both model structure and parameters. There is also an urgent research need for novel uncertainty analysis methods that can accommodate complete error analysis and the Bayesian calibration is one of the most promising prospects (38).

Bayesian calibration can be used to refine our knowledge of model input parameters, obtain insight into the degree of information the data contain about model inputs (i.e., parameter estimates with measures of uncertainty and correlation among the parameters), and obtain predictions and uncertainty bounds for modeled output variables (44, 45). Technically, this method is a proof of the concept that there are better ways to parameterize mechanistic models, other than simply tuning (adjusting) model parameters until the modeler obtains a satisfactory fit. The anticipated technical advances and benefits from the Bayesian calibration would be as follows. (i) *Identification Problem*: By incorporating prior information on the model parameters, the Bayesian inference techniques offer an effective strategy to overcome the identification problem. The use of additional information (along with the calibration dataset) reduces the disparity between what ideally we want to learn (internal description of the system) and what can realistically be observed, which is the primary reason for the poor model identifiability (43). (ii) *Adaptive Management Implementation*: The Bayesian (iterative) nature of the proposed approach is conceptually similar to the policy practice of adaptive management, i.e., an iterative implementation strategy that is recommended to address the often-substantial uncertainty associated with water quality model forecasts and avoid implementation of inefficient and flawed management plans. (iii) *Realistic Uncertainty Estimates of the Ecological Forecasts*: For the purpose of prediction, the Bayesian approach generates a posterior predictive distribution that represents the current estimate of the value of the response variable, taking into account both the uncertainty about the parameters and the uncertainty that remains when the parameters are known (38). Therefore, estimates of the uncertainty of Bayesian model predictions are more realistic (usually larger) than those based on the classical procedures. Predictions are expressed as probability distributions, thereby conveying significantly more information than point estimates in regards to uncertainty (46). The—often deceptive—deterministic statements are avoided and the water quality goals are set by explicitly acknowledging an inevitable risk of non-attainment, the level of which is subject to decisions that reflect different socioeconomic values and environmental concerns.

In conclusion, we examined the factors that determine the recognition (expressed in citation counts) of published studies in the field of mechanistic aquatic biogeochemical modeling. Our analysis provided evidence that modeling papers are cited mainly based on the questions being asked;

models that aim to elucidate oceanic patterns are more highly cited than models developed for addressing local water quality management issues regardless of their methodological features and technical value. While these results cast doubt on the rationale of the current modeling methodology, we suggest that these citation patterns are partly driven by the different practices followed by the two groups of the aquatic ecosystem modeling community. Oceanic modeling evolves more rationally and congruent with the technological constraints and data availability, more easily embraces methodological advances, and more critically considers the future directions. The impressively high number of citations that some of the ocean modeling studies have received, their ability to produce exportable knowledge along with some vital technical improvements (e.g., prudent increase in complexity, rigorous error analysis) dictate what needs to be done to meet the demand for attractive and powerful modeling tools.

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Supporting Information Available

Box 1 - How feasible is the “correct process description”?
Box 2 - What do model parameters represent? This material is available free of charge via the Internet at <http://pubs.acs.org>.

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SUPPORTING INFORMATION

EVALUATION OF THE CURRENT STATE OF MECHANISTIC AQUATIC BIOGEOCHEMICAL MODELING: CITATION ANALYSIS AND FUTURE PERSPECTIVES

**George B. Arhonditsis, Barbara A. Adams-VanHarn, Leah Nielsen,
Craig A. Stow, and Kenneth H. Reckhow**

Box 1: How feasible is the “correct process description”?

Box 2: What do model parameters represent?

Box 1: How feasible is the “correct process description”?

The basic elements of large process-oriented models are simple equations adopted as useful first approximations of isolated behaviors in controlled laboratory experiments. In general, modelers fit a first-order reaction to the behavior, and modified it over time if additional laboratory or field data became available. Although this practice was convenient and necessary to make comprehensive models manageable, it would seem surprising that simple disparate equations should collectively yield useful information about ecosystem behavior. Indeed, we now know that small-scale results may not apply at the ecosystem scale (1).

As an example, consider how modelers have described the mechanism by which nutrients in non-living organic matter are recycled into inorganic forms that are available for phytoplankton uptake and growth. This is a metabolic process by which bacteria degrade particulate organic substrates into soluble substrates and enzymatically assimilate the soluble forms. The rate of mineralization is affected by many factors, including temperature, the physical and biological structure of the organic substrate, and the physiological state of the agents and their enzymatic systems. Organic nitrogen compounds, for example, include proteins, amino acids, amines, nucleotides, and refractory humic compounds of low nitrogen content. Degradation proceeds progressively with different bacteria involved at different stages. Intermediately formed compounds are recycled rapidly; residual forms decompose slowly, being more resistant to utilization by bacteria. Thus, accurate simulation of nutrient mineralization on small time-scales would require complex modeling of specific organic compounds and bacteria to allow for variable mineralization rates. However, the commonly used expressions for mineralization in most water quality models lump organic nitrogen and phosphorus compounds into a single compartment and do not explicitly model bacteria (equations 1.1 and 1.2). What is the scientific basis for these expressions?

$$\frac{\partial ON}{\partial t} = k_{ON} \theta_{ON}^{(T-20)} \{C/(K_m + C)\} ON \quad (1.1)$$

$$\frac{\partial OP}{\partial t} = k_{OP} \theta_{OP}^{(T-20)} \{C/(K_m + C)\} OP \quad (1.2)$$

where ON = organic nitrogen concentration (mg N L^{-1}); OP = organic phosphorus concentration (mg P L^{-1}); k_{ON} = ON mineralization rate at 20°C (d^{-1}); k_{OP} = OP mineralization rate at 20°C (d^{-1}); θ_{ON} = ON mineralization temperature coefficient; θ_{OP} = OP mineralization temperature coefficient; C = phytoplankton carbon concentration (mg C L^{-1}); K_m = half-saturation constant (mg C L^{-1}); T = water temperature ($^\circ\text{C}$); t = time.

First, modelers omitted bacteria because phytoplankton generally have a greater effect on productivity than do bacteria, and the science of metabolic transformations of organic matter was young when the models were initially developed. Second, the equations were constructed to reach a compromise among a series of studies with variable results. Early laboratory studies suggested that degradation of organic matter is reasonably approximated by a first-order reaction, while others suggested second-order models with the recycling rate directly proportional to the phytoplankton. The latter approach seemed reasonable since field studies indicated that bacterial biomass increased with phytoplankton biomass. However, neither first- nor second-order kinetics provided a satisfactory match between observations and expected theoretical results, so Michaelis-Menten half-saturation kinetics were introduced as a compromise between the two. With this factor, the mineralization rate will not increase continuously and is low when the phytoplankton population is low. The result is a manageable expression that has a simple explanation.

The conditions under which equations (1.1) and (1.2) apply are limited by the assumptions upon which they rest. Since these and many other model equations depend to some degree, sometimes completely, on the first-order reaction model, a review of the assumptions required by first-order models is prudent. For equations 1.1 and 1.2 the underlying assumptions are (adapted from 2):

1. All non-living organic nutrient molecules have an identical and independent probability of being

mineralized in a given interval of time.

2. The probability that a given molecule will be mineralized depends only on the length of the interval of time and not when the interval starts.
3. As the time interval is decreased to zero, the probability of mineralization decreases smoothly and continuously to zero.
4. The rate of change of the derivative must be slow relative to the rate at which the underlying elementary events occur; the derivative must be essentially constant during the time interval.

Under what conditions do these assumptions hold true? The first two are violated for relatively small intervals of time because organic nutrient composition is non-homogeneous and degradation is progressive. The fourth assumption is violated for relatively large intervals of time. Models may operate on a variety of time-scales, i.e., the calculation time-step, the output time-step, and the time-step of available data for forcing functions. These time-scales may vary from hours to months. If there was a time interval that can satisfy the above assumptions, and it was within this range, that may explain the usefulness of the first-order model as a first approximation. But how often is this feasible in real world applications?

The limitations described above are typical of the compromises accepted by modelers in their attempts to characterize mechanisms in mathematical models. So, what might we conclude about the mechanisms in process-based models? Of greatest significance, these models are not correctly expressing the mechanisms; thus, the goal or claim that “if the modelers use correct process descriptions then the models can effectively reproduce natural system dynamics” is simply not a reasonable expectation. Beyond that, we seem to be locked into a space/time scale that has become the de facto modeling standard, yet is beyond our ability to correctly capture in the mathematics, and as described in Box 2, is incompatible with available data for parameter estimation.

Box 2: What do model parameters represent?

Model parameters play an essential role in model fit, and yet they rarely can be estimated from site-specific observations. Instead, modelers depend on the scientific and modeling literature for guidance in selecting initial parameter values, which may subsequently be adjusted during calibration. The most common sources of parameter values are model documentation and reference manuals that report plausible ranges of parameter values, list values used in previous model applications, and cite values found in other scientific literature. Among these sources there is a wide range of reported values, sometimes spanning several orders of magnitude. The cause for this variability lies in differences in water bodies, model structures, and measurement conditions that are not always apparent in the literature.

One fundamental difficulty with selecting parameter values from the literature is that experimentally determined values may not be useful because they are often obtained under controlled conditions that do not represent field conditions. As a result, laboratory and field values do not always agree. Lab values of the optimal light intensity for algal growth, for example, are always lower than the values that reproduce observations in the field (3). The discrepancy between laboratory and field values is not surprising, given model nonlinearities and ecological variability. To understand this, suppose that a nonlinear equation of a constituent c is accurate at a point, as in a well-mixed test tube.

$$\frac{\partial c}{\partial t} = kc^2 \quad (2.1)$$

To transfer this equation to a larger body of water, the modeler must assume that there is no variability in c , or that the body is a continuously stirred tank reactor. In practice, the modeler assumes that the equation represents the *average* behavior of the constituent, or that

$$\frac{\partial \bar{c}}{\partial t} = k\bar{c}^2 \quad (2.2)$$

Developing the left-hand side of the equation (2.2) for a fixed number of points in the water body yields:

$$\begin{aligned}
\partial \bar{c} / \partial t &= \partial (\{c_1 + c_2 + c_3 + \dots + c_n\} / n) / \partial t \\
&= 1/n \sum \partial c_i / \partial t \\
&= 1/n \sum k c_i^2 \\
&= k(\bar{c}^2)
\end{aligned}
\tag{2.3}$$

The parameter k cannot satisfy both equations (2.2) and (2.3) unless the variability in c is zero. Since even small compartments of natural water bodies are spatially and temporally variable, experimentally derived values of k may be biased. The inequality between the two equations may be addressed by the use of an “effective” parameter k_{eff} whose value depends on the variability of c over space and time. In practice, modelers use a constant effective parameter value, ignoring system variability. Such values are estimated from a statistical sample of small-scale measurements or by calibrating model predictions to a set of observations by incrementally modifying or “tuning” parameter values to achieve a more satisfying fit between predictions and observations.

Statements in the literature made by modelers in support of their parameter choices are frequently non-informative. For example, parameter choices have been justified because model applications are reported to be “provisional,” or “qualitatively correct”, hypotheses “requiring substantial experimental validation”, or “crude approximations of order of magnitude”. In many cases, parameter values are also justified by favorable assessment of the model goodness-of-fit based on highly aggregated spatiotemporal scales, although the models are actually developed to support predictions at finer scales. Since many ecological properties can be generalized across systems, “reasonable” model results may not be too surprising. However, often a variety of very distinct parameter combinations provide equally good fits between predictions and observations, and optimal parameter choices among these are elusive. Those combinations that will prove most useful in describing aquatic system behavior under different environmental conditions (e.g., external nutrient loading, climate variability) may be impossible to determine *a priori*.

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