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THE NEED FOR INNOVATIVE VERIFICATION OF EUTROPHICATION MODELS*

By

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Introduction

In recent years there has been a trend toward using more mechanistic models of the eutrophication process. By mechanistic, I mean models that account for, or simulate, certain actual processes within the aquatic environment. This excludes models that are only statistical relations between dependent variables, blackbox models that ignore internal dynamics, and models that simulate internal dynamics by unrealistic formulations that are not, or cannot, be measured. These more mechanistic models must follow the same standard procedures of model development, calibration, and verification as have the simpler models; however, as will be discussed below, additional tests may also be necessary to build confidence in application of these models.

The Need for Additional Tests

Often, complete verification of a more mechanistic model is not possible by usual techniques because one does not have a complete and independent data set. This is because sampling all of the properties simulated in more mechanistic models is difficult and expensive (e.g., zooplankton biomass).

Even when a complete verification data set is available and the more mechanistic model has been "verified" by usual techniques, one is left with serious questions concerning reliability for two reasons: 1) calibration and verification tests are subjective and 2) there are increased degrees of

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freedom in these generally nonlinear models. The first reason will not be discussed here because it is considered elsewhere in these proceedings.

The terms increased degrees of freedom, in this context, means that more than one set of coefficient values will satisfy the usual tests for calibration and verification. The basis for increased degrees of freedom is the cyclic nature of mechanistic models. Since these models generally simulate ecosystem cycles, one would not expect material to accumulate excessively in one particular component but rather to flow among all of the components. Then, because of the principles of mass conservation, one could expect that, if the rate of flow were increased or de creased proportionately, the state variable concentrations would not be affected significantly (at least not within the variability usually inherent in the verification data set).

It is for this reason and because of the lack of long-term data that I am suggesting that additional verification tests be included in the standard procedures for testing mechanistic models.

Two Additional Tests

The first type of test is related to gross dynamics and empirical relationships developed for lakes and is particularly useful when long-term verification data are lacking. The second type of test is related to the verification of internal model dynamics and is useful for reducing the degrees of freedom.

Gross properties--If it is impossible or at least very difficult to verify directly the long-term dynamics of the mechanistic model, one can test it indirectly by comparing model output with output from simpler verified models. An example of this approach can be found in Scavia and Chapra (1977). In this study, the results of a mechanistic model were compared with predictions of annual average total phosphorus made by a simple mass-balance model. The mechanistic model (Figure 1) was run to steady-state under a number of nutrient load conditions. At steady-state, annual average total phosphorus was calculated by aggregating the model components and averaging over a year. For the comparison, a simple steady-state mass-balance model for annual average total phosphorus (Dillon and Rigler, 1974a) was solved with the same nutrient load conditions:

$$P = \frac{L(1 - R)}{q_s}, \qquad (1)$$

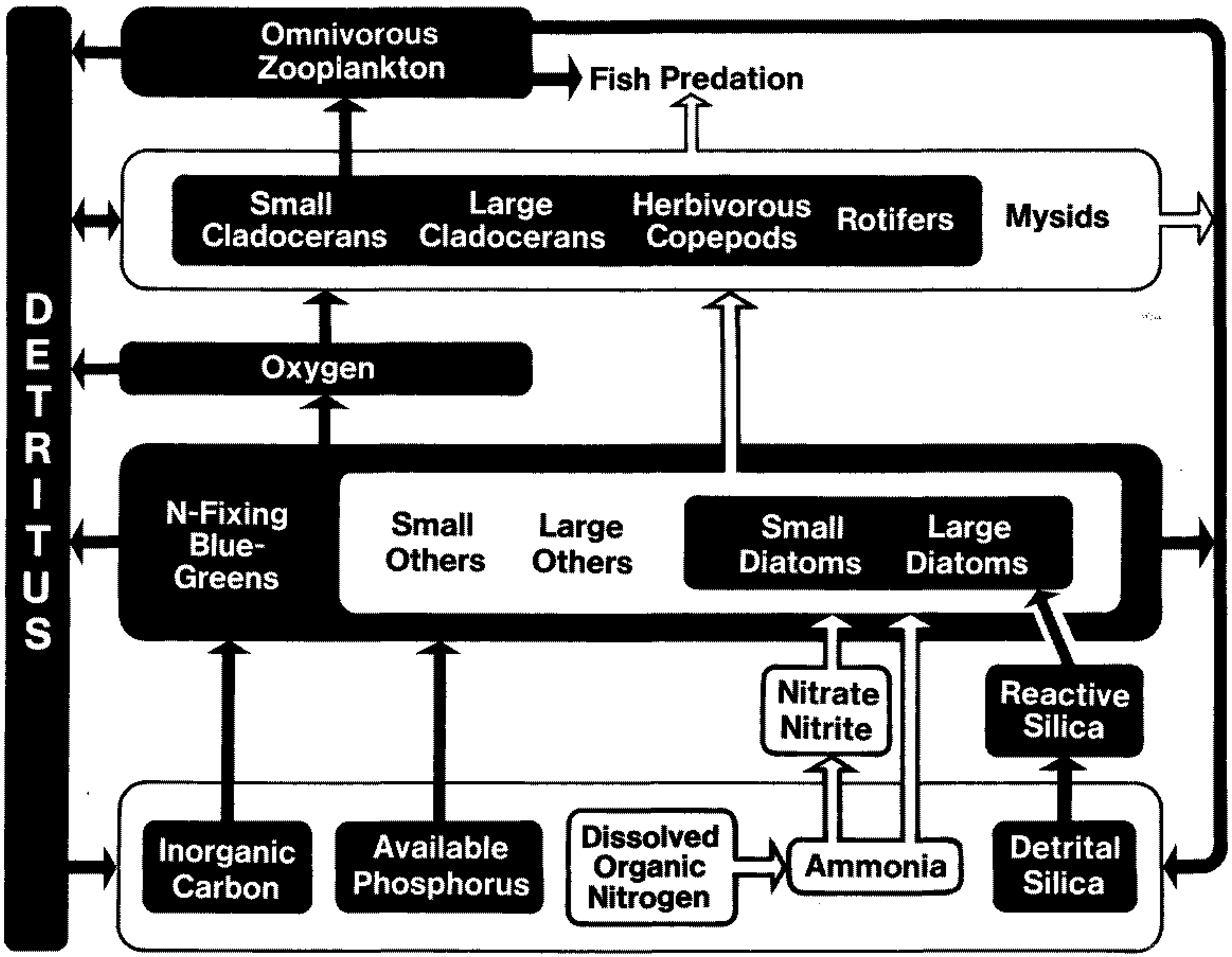


FIGURE I. CONCEPTUAL FRAMEWORK OF MECHANISTIC MODEL

(SCAVIA, 1979a)

where the retention coefficient R is from Chapra (1975):

$$R = \frac{16}{16 + q_s}. \quad (2)$$

Combining equations (1) and (2) yields:

$$P = \frac{L}{16 + q_s}, \quad (3)$$

where P = annual average total phosphorus,
L = phosphorus loading rate, and
q_s = areal water load.

The comparison of the results of the two models (Figure 2) indicates that both produce similar estimates of total phosphorus. Therefore, if the mass balance model was a verified model or was proven to be general in most respects, then the mechanistic model could be considered verified to some degree (at least in terms of long-term mass balance considerations).

Scavia and Chapra (1977) also demonstrated another way to test a mechanistic model in terms of gross properties. In this test, the model output was treated like lake data to see if it conforms to an empirical correlation known to be applicable for a wide variety of lakes. In other words, the model was tested to see if it was behaving like the lake. The correlation (Dillon and Rigler, 1974b) relates (r = 0.95) summer average chlorophyll 'a' (chla) to spring total phosphorus (Pv) for a data set of 46 lakes, each with a nitrogen to phosphorus ratio greater than 12:

$$\log_{10}[\text{chla}] = 1.449 \log_{10}[\text{Pv}] - 1.136. \quad (4)$$

It is reasonable to assume that equation (4) represents well a large cross section of lakes. For model comparison, the mechanistic model (Figure 1) was run under a number of conditions, and for each year that N:P>12, spring total P concentrations and summer average chlorophyll 'a' concentrations were calculated. These results were then plotted (Figure 3), along with equation (4). The agreement between model output and the empirical curve was good up to a point. Beyond about 75 μgP/l, the model output diverged consistently from the line. Thus, in this case, confidence in the model was inspired because it reproduced the relationship between spring phosphorus and summer chlorophyll 'a'; however, other important information was also obtained. The model failed to function consistently under extremely eutrophic conditions. Scavia and Chapra (1977) suggest causes for the failure, but the important point here is that

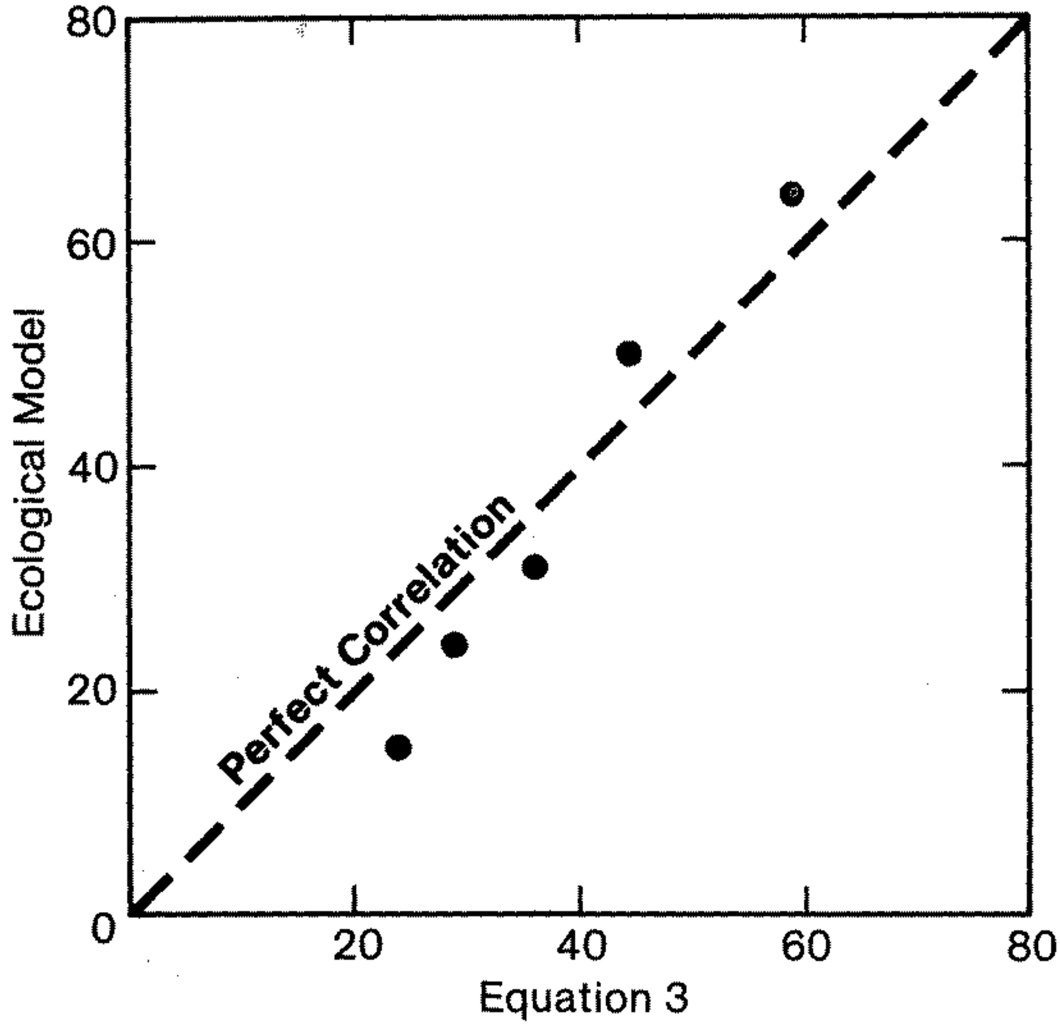


FIGURE 2. COMPARISON OF TOTAL PHOSPHORUS CONCENTRATION (mg/m^3) AS CALCULATED BY THE MECHANISTIC MODEL AND BY EQUATION (3)

(SCAVIA AND CHAPRA, 1977)

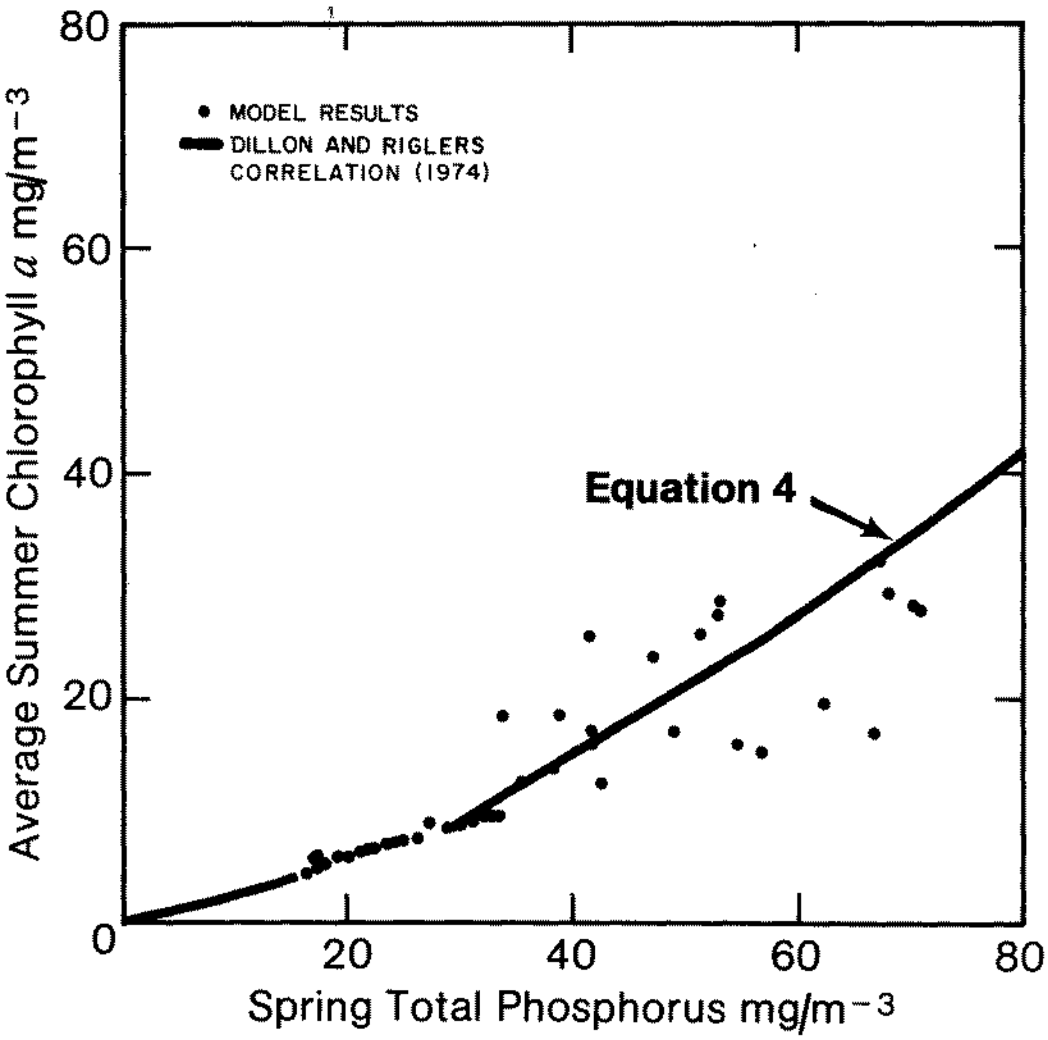


FIGURE 3. COMPARISON OF MECHANISTIC MODEL RESULTS AND CORRELATION LINE BETWEEN AVERAGE SUMMER CHLOROPHYLL a AND SPRING TOTAL PHOSPHORUS

(SCAVIA AND CHAPRA, 1977)

this verification procedure provided a test of confidence as well as set a possible limit to the model's applicability.

Internal dynamics--The second type of verification test proposed here is verification of the internal dynamics of the mechanistic model. One of the most important reasons for using mechanistic models is to examine the controls of the system. For example, a mechanistic model can be used to examine the controls of phytoplankton production (Figure 4) and phosphorus cycling (Figure 5). In this context, model output is used to estimate the timing and relative magnitude of the influence of specific processes on state-variable dynamics. One important question concerning this use of the model is whether the simulated process rates are accurate representations of real processes. As mentioned above, compensating errors at the process level might lead to a successful calibration at the state-variable level. Thus, if models are to be used at the process level and we are to have faith in the dynamics that produce the state-variables, we must look closely at the modeled processes.

The following example demonstrates one method of verifying processes and the way in which compensating errors at the process level can lead to erroneous conclusions regarding system controls.

After initial calibration of the state variables in a mechanistic model of Lake Ontario (Figure 1), simulated process rates were compared to actual measurements. For this comparison, a summer averaged (July-Sept.) phosphorus flow diagram was constructed (Figure 6a) from aggregated model output. The flow (or transfer) rates were then compared to measurements and calculations from Lake Ontario and to other, more theoretical estimates. Many of the simulated process rates were very low (as much as 3-7 times lower) compared to actual rates, with the most serious discrepancies in transfers among available phosphorus, phytoplankton, and zooplankton, yet the state variables compared successfully! Therefore, I calibrated the model again, keeping the process rates in mind and most coefficient values still within acceptable ranges. The new calibration is shown in Figure 6b. The interesting point here is that the state variables are close to the originally calibrated values and can still be considered calibrated; however, the process rates are much higher and, in fact, much closer to observed values (Scavia, 1979b).

This example demonstrates that if the model were calibrated only in terms of state variables and then used to examine control of the phosphorus cycle, then the relative importance of certain processes would be overestimated by almost an order of magnitude. For example, bacterial regeneration of available phosphorus (detritus available P) is relatively more important in Figure 6a than in Figure 6b and the relative

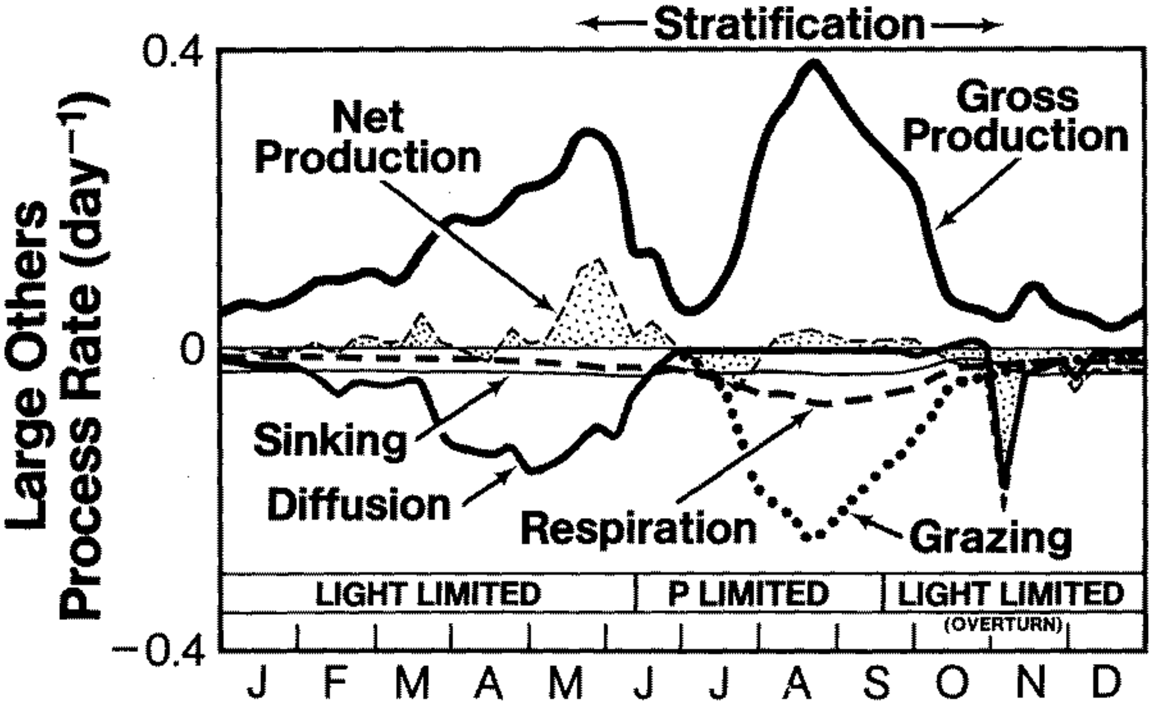


FIGURE 4. RATE PLOT INDICATING SIMULATED CONTROLS OF EPILIMNION PHYTOPLANKTON DYNAMICS IN LAKE ONTARIO

(SCAVIA 1979b)

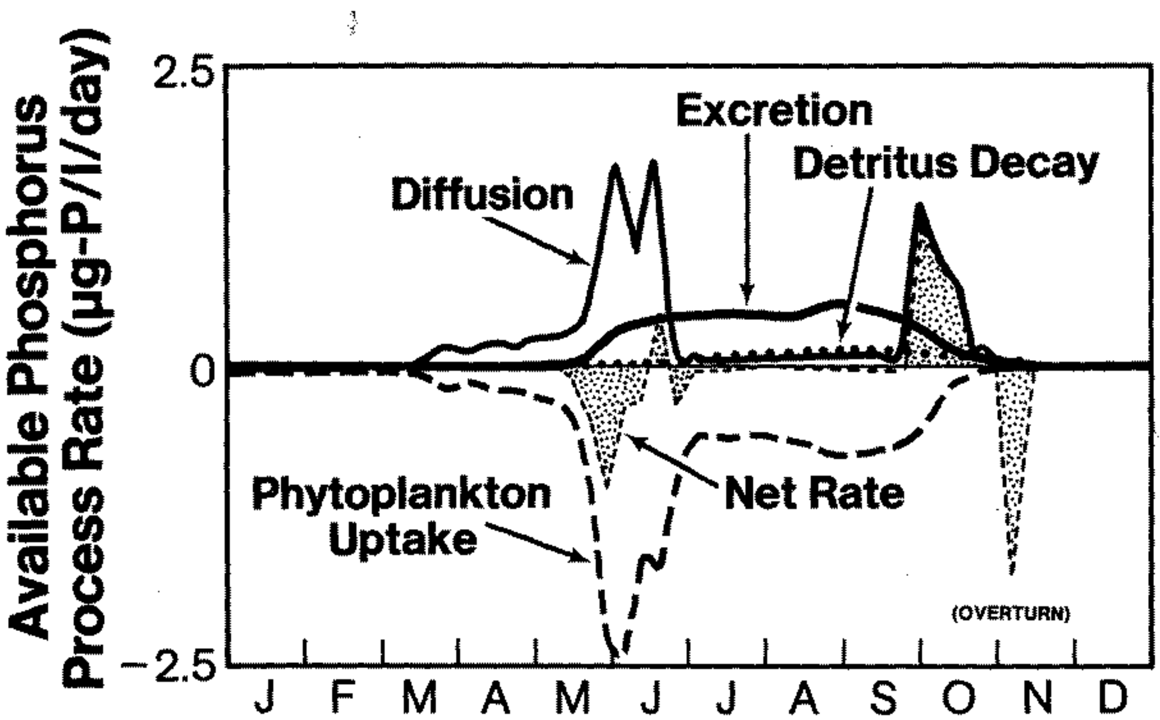
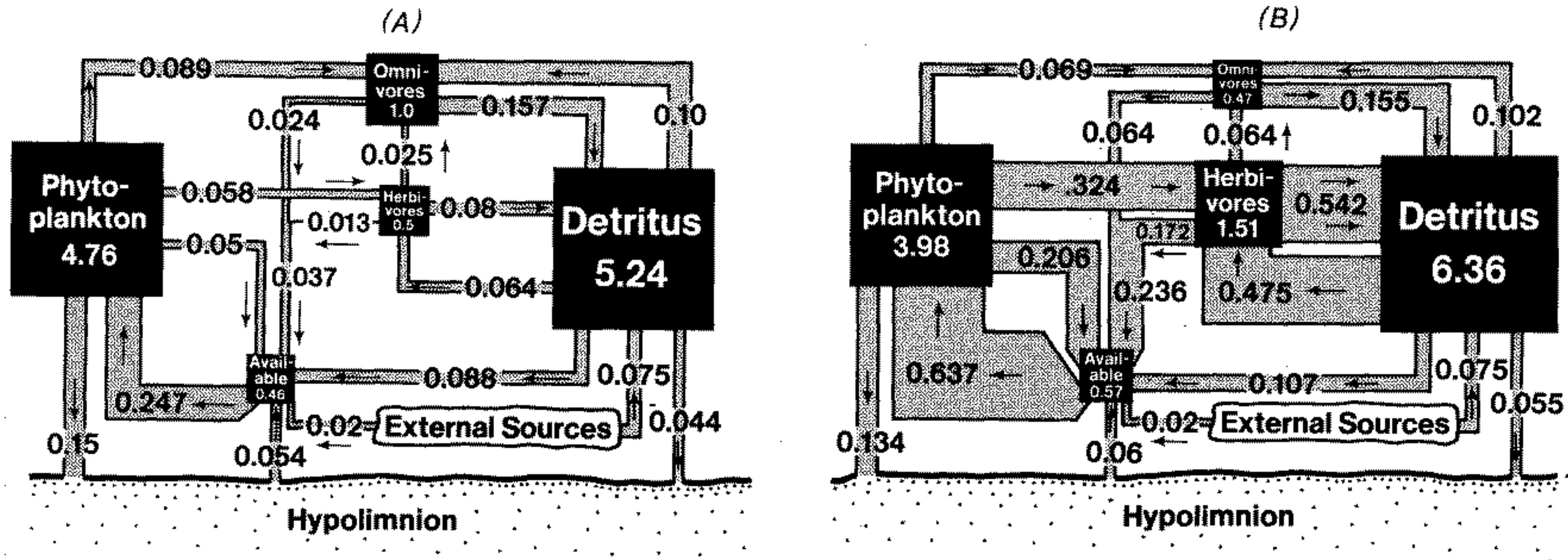


FIGURE 5. RATE PLOT INDICATING CONTROL OF PHOSPHORUS DYNAMICS

(SCAVIA 1979b)

STATE VARIABLE CALIBRATION

STATE VARIABLE AND PROCESS CALIBRATION



NOTE:
CONCENTRATIONS IN BOXES ARE IN μg-P/L
CONCENTRATIONS IN PIPES ARE IN μg-P/L/DAY

FIGURE 6. PHOSPHORUS FLOW DIAGRAM

importance of external loads and of transport into and out of the epilimnion is exaggerated in Figure 6a.

Summary

Because of increased degrees of freedom and the usual lack of longterm verification data, mechanistic models need verification tests beyond the standard tests used for state variable simulation. Two general types of verification can be useful additionals to the usual tests: 1) a comparison of aggregated output from the mechanistic model with output from simpler models and empirical correlations that have been verified or proven to be general and 2) a comparison of simulated process rates with rates measured in the field or in the laboratory to determine if the model's internal dynamics are consistent with measured and theoretical dynamics.

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