Variance Estimates for a Dynamic Eutrophication Model of Saginaw Bay, Lake Huron

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First-order variance propagation is used to estimate variance of model output originating from variances of uncertain initial conditions, parameter values, and external load estimates for a nutrient-phytoplankton-zooplankton dynamic eutrophication model of one segment of Saginaw Bay, Lake Huron. Coefficients of variation of model output during summer are not unlike those estimated from measurements. The major source of variance is parameter value variances. The most important parameters, in terms of model sensitivity and variance propagation, are identified by analysis of the predicted correlation matrix. Methods for reducing model output variance are suggested.

INTRODUCTION

Mathematical modeling of aquatic ecosystems has become a relatively common tool in management contexts. In many cases, it has also become useful for suggesting research needs, synthesizing extant information, and analyzing these ecosystems in ways that are not tractable through field and laboratory studies alone. The models used most often in these contexts have similar attributes; they are generally time-dependent, often nonlinear, ordinary differential equation models based on parameterized physiological processes and mass conservation.

These models, whether from the management or the research milieu, have another common thread: they are generally deterministic. That is, although it is often recognized that model initial conditions, parameters, and forcing functions are stochastic, this is seldom accounted for. Moving beyond acknowledgment of variances of these elements to assessment of their effects is important because these stochastic properties affect the confidence that can be placed in the model output; that is, confidence is generally inversely related to variance.

Analysis of this variability is important in a management context to establish error bounds on predictions. Eutrophication models have been developed to generate deterministic predictions of water quality based on present and expected scenarios of system inputs [e.g., DiToro et al., 1971; Chen and Orlow, 1975; Thomann et al., 1975, 1976, 1979; Canale et al., 1976; Bierman, 1976]. Output from these deterministic models often influences decisions affecting many thousands of people socially and economically [e.g., Valente and Thomas, 1978]; yet quantitative limits of confidence are lacking for these models [Mueller, 1986], unlike many of their simpler counterparts [e.g., Chappell and Reckhow, 1979; Reckhow, 1979; Latenmate and Richey, 1979; Reckhow and Simpson, 1980]. In particular, only qualitative evaluations of calibration and verification results have been carried out to date, and experience with even these tests is limited. Because eutrophication models are crude representations of highly variable, stochastic systems, ignoring such important attributes often results in naive confidence or unwarranted disbelief in the models' solutions. For these models to become more generally accepted and effectively used, they must be placed in their proper perspective. Evaluating the effects of input (forcing function and parameter) variability on model output provides some of the needed perspective.

Analysis of model variability is also important in research contexts where a model's ability to simulate must be evaluated prior to investigation of specific system properties and recognition of actual system variability is important. Models have recently been used as data synthesizers and as tools for detailed ecological systems analysis [e.g., Lehman, 1978; Robertson and Scavia, 1979; Scavia, 1979a, b; Halfon, 1979; Scavia and Bennett, 1980]. Output from these models is often used to assess the relative importance of various system compartments or processes and thus to focus additional effort on key problems. Prior to using a model in this context, it is important to evaluate its ability to function as a synthesizer or interpolator. Traditionally, this evaluation is done by comparing model and measurement trajectories, with no quantitative assessment of model or measurement variability. It has been demonstrated that comparison of modeled and measured state variables alone is not sufficient for this purpose [Scavia, 1980b]. Calculation of variance associated with model state variables and of correlations among state variables and parameters will assist in evaluation of these models for use in research contexts.

The need to assess model output variability results in two problems. The first is the need to establish a method by which model output variance can be estimated. The second deals with estimating that variance and identifying its major sources. The method used for variance estimation herein, first-order variance propagation, was compared to Monte Carlo analysis [Scavia et al., this issue]. The comparisons suggested that variance estimates from the two techniques were similar qualitatively; however, differences were attributed to different interpretation of variance from the two approaches.
First-order analysis measures variability about the deterministic model trajectory. This is the quantity of interest herein. The present paper is concerned with the second problem, i.e., (1) application of the above method to estimate variance of model output based on variable initial conditions, parameters, and loads and (2) evaluation of the most significant sources of variability, given those estimates.

Several recent works [e.g., O’Neill, 1973; O’Neill and Gardner, 1975; Gardner et al., 1980b; O’Neill et al., 1980] explore errors in typical ecological models and submodels. These papers provide an excellent framework for such analyses and illustrate potential contributions to overall error from various sources. Herein we provide an error analysis of a previously developed eutrophication model applied in a real world situation.

In the following sections of this paper, first-order variance propagation and the Saginaw Bay eutrophication model are described, a summary of the variances of input and the resulting model output are given, and the most significant sources of that variance are identified.

Methods

The Model

The system model used herein was developed for predicting trends of eutrophication in large lakes. Developed originally for Lake Ontario [Thomann et al., 1975, 1976], it has been modified and applied in several other contexts [Canale et al., 1974; DiToro and Majystik, 1976, 1979, 1980; Richardson and Bierman, 1976; Thomann et al., 1977]. The model is an eight-state-variable, nonlinear, time-dependent food chain model designed to simulate seasonal dynamics in one vertically averaged inner portion of Saginaw Bay, Lake Huron [see Scavia et al., this issue]. The model simulates dynamics of phytoplankton, herbivorous and carnivorous zooplankton, three chemical forms of nitrogen, and two chemical forms of phosphorus. The general interactions among state variables and examples of nonlinear formulations are illustrated conceptually by Scavia et al. [this issue]. Detailed model equations, parameter values, and references to boundary conditions, forcing functions, and driving data are given by Scavia [1980a], Bierman et al. [1980], and Thomann et al. [1975]. The model was calibrated, by manipulation of parameter values, to the 1974 data set (Figure 1).

First-Order Variance Propagation

The equation used for estimation of propagated variance in the nonlinear, continuous-dynamics case is the following matrix differential equation for covariance [Gelb, 1974]:

\[ \dot{P} = AP + PA^T + Q \]  

where \( Q \) is the model equation noise, variance-covariance matrix, \( P \) is the augmented variance-covariance matrix of state variables and parameters, and

\[ A_{ij} = \frac{\partial g_i}{\partial x_j} \]

where \( g_i \) is the model equation for the \( i \)th state variable and \( x_j \) is the \( j \)th state variable or parameter.

In the present analysis the equations were assumed to be known perfectly; thus \( Q \) was set equal to zero (except as noted below). The approximation \( A \) of the nonlinear state dynamics is derived from a first-order Taylor series approximation of the model about the current estimate of the state variables. Thus the matrix \( A \) is evaluated at the current values of \( X \) during the simulation. In this application the partial derivatives were calculated analytically. Because \( A \) represents the time progression of state variables, it is clear that propagated variance will be controlled, not only by initial variances and covariances of state variables and parameters \( P(0) \), but also by the model dynamics \( A \). Thus as demonstrated below, variance can both build and decay in time.

A brief discussion of this method and its relationship to the present model is given by Scavia et al. [this issue]. Details concerning the derivation and a review of previous applications are given by Gelb [1974] and Scavia [1980a], respectively. In this procedure, effects of parameters on state variables are included by augmenting the original state variable system with stochastic differential equations describing the parameters [see Gelb, 1974, sec. 9.4]. Unlike first-order sensitivity analysis, first-order variance propagation includes not only the simultaneous effects (sensitivity) of all state variables and concerned parameters on each state variable but also the propagation of the variances of those parameters and state variables. Therefore this analysis does not examine the effects of only one parameter at a time. Also, parameter importance, as well as other error sources, are judged finally in terms of both their sensitivity and uncertainty.

The matrix differential equation for \( P \) and the state-variable equations were solved by numerical integration with a paired 5th-6th order Runge-Kutta method [International Mathematical and Statistical Libraries, 1977].

Input Statistics

Sources of variability whose effects may propagate through the model can be grouped into four categories: (1) initial conditions, (2) parameters, (3) inputs or forcing functions, and (4) model equations. Variability within the first and third category is often measured and quantified (e.g., mean and variance). Statistical distributions of parameter values have not been determined generally. However, recent works have examined some parameters, and their variability can be defined, at least in terms of ranges, from the literature. There has not been a thorough examination of variability or uncertainty inherent in the model equations themselves. Experience with the models and knowledge of the adequacy of the individual theories and assumptions upon which they are built will allow assessment of relative confidence in model equations, at least qualitatively.

In this particular application the following were assumed as sources of variance: (1) 7 of the 22 parameters, (2) all of the 8 initial conditions, (3) all of the 5 nutrient loads, and (4) the mixing parameter at the boundary between inner and outer bay segments. It was assumed that the remaining 15 parameters and the model equations were perfect deterministic functions; a rationale for selecting the 7 uncertain parameters is discussed below. (Actually, some model-equation variance is represented as parameter variance because model equations were often used to normalize literature values that were determined under diverse conditions.) The variability associated with initial conditions, parameters, and loads is a representation of natural variability and not of errors inherent in measurement. Measurement errors are not included because in this application they are generally much smaller than natural variability. For example, because of spatial heterogeneity in the bay, coefficients of variation (CV) for the mean of sampling stations in inner Saginaw Bay were always much larger than measurement errors. The same was true for loading estimates, except that in this case the variability was temporal.
Variability in parameter values was due less to errors in measurement than to errors associated with representing a highly diverse system with relatively simple parameterizations specifically simulating a group of organisms or chemical species by their typical characteristics. Variance associated with the mixing parameter was not due to measurement error or natural variability because it was not a measured value but rather a calibrated parameter. Thus its variance is more a statement of faith in its calibration.

Treating input errors as done herein allows estimates of model variance that correspond to variance of the natural system. It does not strictly estimate the error associated with the ability of the model to predict. To do this, one certainly must examine errors introduced by the equations themselves and perform the analysis over the time frame of the prediction, as has been done for some empirical and simpler lake models [e.g., Reckhow, 1979]. However, because variance due to measurement errors is small compared to natural variability in this system, these variance estimates measure at least their contribution to prediction variances.

Variance of initial conditions (February 20, 1974) was estimated by calculating the sample variance of measurements.
from all depths at all stations in the inner bay. For the cases where the state variables were not measured until a later date, variance was estimated from coefficients of variation from other winter sampling dates. Initial-condition means and variances are shown in Table 1.

Variance associated with loading estimates was calculated from time-variable loads multiplied by coefficients of variance of stratified (partitioned in time) samples because loading variability was much higher in the early part of the year. Externally loaded model equations as simple bias terms: \( x = g(x, t) + L/V, L = \text{load (g m}^{-1} \text{ day}^{-1}) \), and \( V = \text{volume (0.806 X 10}^{10} \text{ m}^3) \). Therefore loading variance was included along the diagonal of the matrix \( Q \) in (1). The coefficients of variation of this bias term for each load and each of the two time strata are shown in Table 2.

Variance estimates for the seven parameters (defined in Table 3) were obtained from several sources. Recently, Canale et al. [1974], Ford et al. [1976], Zitson et al. [1978], and Jorgensen [1979] have published extensive literature reviews of parameter values. In addition to these surveys, additional reviews were conducted and results reported by Scavia [1980a]. Summaries of parameter statistics from each review and values used herein are listed in Table 4. We assumed the variances were not time dependent. These particular parameters were selected for two reasons. In terms of model sensitivity, experience has demonstrated that these parameters are more 'important' than others. A second criterion was availability of information from which parameter statistics could be generated. Including a parameter whose variance had to be assumed arbitrarily made little sense. However, one must be aware that this implies perfect knowledge (i.e., zero variance) of those parameter values. This is one reason why we used overestimates of variance for parameters included in the analysis. These variances are probably overestimates because they were calculated generally from all available literature values with little regard for differences in experimental conditions. If parameter values were collected only for 'eutrophic species' of phytoplankton, for example, one would expect the variance to be lower than if it were calculated from a broader spectrum of species.

In several studies on Saginaw Bay, horizontal mixing has been examined. DiToro and Matsyuk [1980] considered mixing at the Saginaw Bay-Lake Huron interface. Bieman and Dolan [1976], Bieman [1976], and Bieman et al. [1980] considered mixing between inner and outer bay segments. Mixing characteristics and transport have also been examined for S-segment [Richardson and Bieman, 1976], 16-segment [Rich-
simulation and suggest, from that perspective, that sampling during summer is not particularly useful for model validation. Moore [1973] and Moore et al. [1976] present excellent strategies for design of water quality sampling programs based on estimation and subsequent reduction of variances. It is of interest then to determine the most significant sources of variability in this model. From the standpoint of model variance the relative effects can be demonstrated easily. In the simulations discussed below, initial condition, parameter, load, and mixing parameter variances were each used singly or in simple combinations.

Assuming perfect knowledge of initial conditions reduced maximum output variances only slightly. Conversely, assuming uncertain initial conditions and perfect knowledge of parameter values resulted in much lower errors. Thus parameter variance contributes far more than initial-condition variance. (See first 3 lines of Table 6.) Variance associated with loadings contributed little, even when compared to the low initial-condition contribution (line 4, Table 6). Noise of the CV increased more than 20% when loading variances were included. In fact, only ammonia-nitrogen (NH₃-N) and nitrate-nitrogen (NO₃-N) CV increased more than a few percent. Including uncertainty (CV = 10%) in the mixing parameter also had little effect (line 5, Table 6). In fact, even when its

### TABLE 3. Parameter Values Assumed Uncertain in Saginaw Bay Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Definition</th>
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</thead>
<tbody>
<tr>
<td>KIC</td>
<td>0.58</td>
<td>day⁻¹</td>
<td>maximum phytoplankton specific growth rate</td>
</tr>
<tr>
<td>KMP</td>
<td>0.005</td>
<td>mg P l⁻¹</td>
<td>Michaelis constant for phosphorus</td>
</tr>
<tr>
<td>CGT</td>
<td>0.06</td>
<td>1 mg C⁻¹ day⁻¹ °C⁻¹</td>
<td>herbivorous zooplankton filter rate</td>
</tr>
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<td>CCHL</td>
<td>30.0</td>
<td>mg C mg Chl⁻¹</td>
<td>carbon to chlorophyll ratio</td>
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<td>KMPL</td>
<td>0.02</td>
<td>mg l⁻¹</td>
<td>Michaelis constant for phytoplankton</td>
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<td>K4T</td>
<td>0.005</td>
<td>(day °C)⁻¹</td>
<td>herbivore respiration rate</td>
</tr>
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<td>PCHL</td>
<td>0.6</td>
<td>mg P mg Chl⁻¹</td>
<td>phosphorus to chlorophyll ratio</td>
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### TABLE 4. Statistics for Parameter Values

<table>
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<tr>
<th>Variable</th>
<th>Coefficient of Variation</th>
<th>Mean</th>
<th>Variance</th>
<th>Number</th>
<th>Source</th>
<th>Comment</th>
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<td>KIC</td>
<td>0.057</td>
<td>0.64</td>
<td>0.057</td>
<td>37</td>
<td>26</td>
<td>Canale et al. [1974]</td>
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<td>diatom</td>
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<tr>
<td>KMPL</td>
<td>0.0075</td>
<td>0.053</td>
<td>0.0075</td>
<td>163</td>
<td>14</td>
<td>Scavia [1980a]</td>
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<td>Bosmina, Diaptomus, Daphnia</td>
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<td>Bosmina only</td>
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<tr>
<td>CGT</td>
<td>0.0063</td>
<td>0.022</td>
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<td>8</td>
<td>Scavia [1980a]</td>
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<tr>
<td>K4T</td>
<td>0.0043</td>
<td>0.016</td>
<td>0.00043</td>
<td>72</td>
<td>17</td>
<td>DiToro et al. [1971]</td>
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<td>Cladocera</td>
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<td>assumed at 20°C, 0.01</td>
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<td>mg C individual⁻¹</td>
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<tr>
<td>PCHL</td>
<td>0.000157</td>
<td>0.033</td>
<td>0.000157</td>
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<td>4</td>
<td>Weitzel [1975]</td>
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<tr>
<td>CCHL</td>
<td>0.002</td>
<td>0.06</td>
<td>0.002</td>
<td>75</td>
<td>13</td>
<td>Weitzel [1975]</td>
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<tr>
<td>KMP</td>
<td>0.002</td>
<td>0.012</td>
<td>4 x 10⁻⁵</td>
<td>54</td>
<td>33</td>
<td>DiToro et al. [1971]</td>
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<td>assume O₂, C = 2.75, maximum</td>
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<tr>
<td>PCHL</td>
<td>0.0001</td>
<td>0.016</td>
<td>0.0001</td>
<td>49</td>
<td>48</td>
<td>Zitson et al. [1978]</td>
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<tr>
<td>CCHL</td>
<td>0.005</td>
<td>0.006</td>
<td>100</td>
<td>100</td>
<td>42</td>
<td>Jorgensen [1979]</td>
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</tr>
<tr>
<td>KMP</td>
<td>0.0075</td>
<td>0.007</td>
<td>3.7 x 10⁻⁵</td>
<td>81</td>
<td>14</td>
<td>Canale et al. [1974]</td>
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<td>Ford et al. [1978]</td>
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<tr>
<td>PCHL</td>
<td>0.005</td>
<td>0.005</td>
<td>6 x 10⁻⁶</td>
<td>49</td>
<td>49</td>
<td>Jorgensen [1979]</td>
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TABLE 5. Maximum and Mean of Summer Coefficients of Variation (Percent) Calculated by the First-Order Analysis From Uncertain Initial Conditions and Parameters Compared to Coefficients of Variation From Measured Variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Maximum Mean</th>
<th>Summer Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phytoplankton</td>
<td>593 78</td>
<td>52</td>
</tr>
<tr>
<td>Herbivores</td>
<td>772 206</td>
<td>65</td>
</tr>
<tr>
<td>Organic N</td>
<td>148 33</td>
<td>48</td>
</tr>
<tr>
<td>Ammonium</td>
<td>201 155</td>
<td>92</td>
</tr>
<tr>
<td>Nitrate-nitrite</td>
<td>550 407</td>
<td>40</td>
</tr>
<tr>
<td>Organic P</td>
<td>163 48</td>
<td>96</td>
</tr>
<tr>
<td>PO4</td>
<td>552 186</td>
<td>115</td>
</tr>
<tr>
<td>Carnivores</td>
<td>707 266</td>
<td>67</td>
</tr>
</tbody>
</table>

*Summer: July-September.
†Calculated coefficient of variation of spatially averaged values from all sampling dates.

Assumed variance was doubled, no state-variable maximum CV increased more than 1%. These results are consistent with more detailed analyses performed on an ecologically simpler, two-segment model [Scavia, 1980a].

Recall that loading variance represents time variability only. It is well known that estimating loads from highly variable, episodic inputs is difficult. To examine the potential influence of these inadequacies, two more cases were run, 2 and 10 times the load variance, respectively. These runs assume that loading standard deviations other than temporal are equal to that due to temporal variability and equal to 3 times that variability, respectively. Dilution effects of the inner bay (volume = 10^9 m^3) somewhat mitigated even this variability when compared to variance propagated from initial-condition and parameter sources (lines 6 and 7, Table 6). The largest effects were seen in the CV for NH3-N and NO3-N; increasing load variances by a factor of 10, an extreme case, resulted in doubling their model-output standard deviations.

These tests of the relative effects of different variance sources on propagated variances for a 1-year simulation indicated that parameters were by far the most significant contributors. The effects of initial-condition variance were quickly surpassed by the effects of parameter variance during the simulation, and only when very large loading measurement errors are assumed do load variances contribute significantly. We did not examine results of errors propagated over longer than the 1-year time frame. If we were examining long-term prediction errors, the effects of uncertain load predictions (not measurements) would have to be considered. This would certainly increase the variance contribution of loading estimates.

The relative effect of individual parameters was also examined. In these tests, the estimated covariance matrix, as well as its changes during the annual simulation, were examined. Recall that the covariance matrix P included parameter variances and their estimated covariances with state variables. This covariance matrix was examined to reveal significant relationships between parameters and state variables. Differences in individual variance magnitudes required scaling covariances, and this was done by calculating the correlation matrix from the covariances. This procedure scales elements of the covariance matrix to between 0.0 and 1.0. Correlation coefficients reveal only linear trends; however, as the correlation matrix changed character during the annual simulation, the changing of important parameters reflected time variability of model dynamics. The procedure is a type of sensitivity analysis that considers all parameter effects simultaneously and employs both sensitivity (i.e., dS/dx) and parameter variance to determine important state variable-parameter pairs. [Gardner et al. 1980a, b] caution and demonstrate that sensitivity analysis without consideration of parameter variance cannot produce misleading information regarding the importance of specific parameters as contributors to model variance.

Typical correlation matrices from two time segments (Table 7) illustrate the magnitudes and shifts in dominant correlations. For example, on day 141, phytoplankton and available phosphorus (PO4) were highly correlated (p = 0.81), while phytoplankton and nitrate (NO3) were less correlated (p = 0.42). Later in the year (day 239) the situation reversed: phytoplankton-phosphorus correlation (0.31) was overshadowed by phytoplankton-nitrate correlation (~0.70). This shift accurately reflects the control of phytoplankton production from phosphorus to nitrogen limitation. The high correlation among most state variables also illustrates their close coupling.

More important in the present context are the correlations between state variables and parameters. These are illustrated in the lower seven rows of the correlation matrix. (The 15 x 15 matrix is incomplete in this table because, under the assumptions of the model, the parameters are independent; thus correlation among them is zero.) Again, as illustrated for the two dates in Table 7, different parameters were important at various stages in the simulation. [Gardner et al. 1980a, b] and O'Neill et al. [1980] also observed changes in importance of certain parameters with time in nonlinear ecosystem and hydrology models. Here, zooplankton grazing (CGT) and the plankton-carbon-to-chlorophyll ratio (CCHL) appeared im-

TABLE 6. Estimated Maximum Coefficients of Variation (Percent) with Different Variance Sources

<table>
<thead>
<tr>
<th>Variance Sources</th>
<th>Phytoplankton</th>
<th>Herbivores</th>
<th>Organic N</th>
<th>NH3</th>
<th>NO3</th>
<th>Organic P</th>
<th>PO4</th>
<th>Carnivores</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial condition only</td>
<td>38 81</td>
<td>24 46</td>
<td>123 536</td>
<td>163 348</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameters only</td>
<td>592 768</td>
<td>148 196</td>
<td>201 550</td>
<td>163 552</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameters and initial conditions</td>
<td>593 772</td>
<td>148 201</td>
<td>550 163</td>
<td>552 707</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Initial conditions and loads</td>
<td>38 81</td>
<td>25 55</td>
<td>148 26</td>
<td>60 59</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Initial conditions, loads, and mixing parameter initial conditions, loads</td>
<td>38 81</td>
<td>25 55</td>
<td>151 26</td>
<td>61 60</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>×2, and mixing parameter initial conditions, loads</td>
<td>39 82</td>
<td>26 63</td>
<td>172 28</td>
<td>63 61</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
<tr>
<td>×10, and mixing parameter initial conditions, loads</td>
<td>41 84</td>
<td>33 106</td>
<td>291 43</td>
<td>81 69</td>
<td>58 704</td>
<td>707</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
important to most state variables on day 141, whereas later in the simulation (day 239), correlations with the plankton phosphorus-to-chlorophyll ratio (PCHL) dominated in many cases.

Correlation matrices were examined throughout the period of simulation and general tendencies were observed. Figure 2 maps the results of these observations as important parameters ($|r| > 0.5$) in time and state-variable space. Some clear patterns emerge: (1) Early in the simulation, phytoplankton growth rate (KIC) dominated as the most important parameter. (2) During late spring to midsummer, CGT and CCHL dominated. These two parameters remained most important for the food chain variables (phytoplankton, herbivores, carnivores) throughout the simulation. (3) The phosphorus state variables became correlated most highly with the phosphorus-to-chlorophyll ratio (PCHL), and that parameter remained dominant from midsummer through the end of the simulation. (4) PCHL also became important to the nitrogen state variables, but it was replaced by KIC, CGT, and CCHL during the last 3 months of the year. (5) Two other parameters appeared important for only short periods of time. The zooplankton feeding efficiency parameter (KMPL) influenced the two organic nutrient states, and the herbivorous zooplankton respiration rate (K4T) influenced the herbivores for a short time. These interrelationships reflect both correlations between parameters and state variables and significant variance contributions from individual parameters.

**Discussion**

The propagation of variance discussed herein is similar to the analysis of predictability in meteorology in that it estimates the extent to which stochastic (or uncertain) inputs corrupt the deterministic aspects of model output. A particularly interesting attribute of this eutrophication model analysis is that variances appear bounded; that is, dynamics of the model equations force both growth and decay of variance, unlike the meteorological counterparts whose imperfect initial conditions tend to eventually overtake the prediction in time [see Holton, 1972]. Gardner et al. [1980a, b] found hydrology and ecological model output variances to be bounded. The stability of errors in these models is clearly tied to model dynamics that cause both growth and decay of state variable values and errors. Gardner et al. [1980b] attribute the bounded error to environmental constraints which, in their case, caused derivatives of state variables to change from positive to negative. In general, any property of the model causing such sign changes will be effective. In our simulations, interactions among state variables themselves contribute largely to those dynamics.

The relatively stable variance prediction for these models may be tied to the assumption of error-free equations. That is, if model structure error is included in the analysis, model variance will also increase unbounded in time (provided structure error does not diminish in time). The rate at which these errors grow depends on the magnitude of equation error, which, at this time, is largely unknown.

In the above analysis, initial-condition variances (estimated from measurement sample variance) and parameter variances (estimated from compilation of literature values) were input to the variance-propagation equations, and resultant state-variable variances were compared to variances of Saginaw Bay data. Maximum CV for simulated phytoplankton was 593%; the average CV of simulated summer phytoplankton was 78%. While the maximum CV was quite large, the summer average CV was not much greater than the annual average CV of phytoplankton measurements (52%). The average
summer model CV for all eight state variables ranged between 33 and 407%, whereas the average annual CV of measurements ranged between 40 and 115%. This demonstrated that after spring, the simulation variances were generally comparable to data variances. One notable exception is the poorly simulated carnivorous zooplankton. The general agreement is especially true if the CV for simulated NO3-N (467%) is not considered; the remaining simulation CV ranged between 33 and 266%. The fact that the CV of measured and simulated variables are comparable during summer may indicate that the confidence intervals of both the spatially averaged measures and the model output each include approximately the same portion of the theoretical total population of samples in the bay. This is true if the model equations are error free and if the input variance sources considered here are the only important sources.

The large CV for the spatially averaged measurements is due in large part to spatial gradients in the bay; therefore if one divides the inner bay into subsections, as Richardson and Bierman [1976] and Canale and Squire [1976] did, the CV of observations will be smaller. Also, the assumptions of error-free equations and no other significant variance sources are surely not completely acceptable. For these reasons the relative contributions of the assumed sources of model variance were examined to determine which were most significant, indicating which sources could be used most effectively to reduce model output variance. Results demonstrated that parameter variance far outweighed that originating from initial conditions, loads, and the mixing coefficient. This implies that the most dramatic reduction in output variance can be affected through reducing parameter variance.

Parameter variance can be reduced in several ways. One way is to aggregate model state variables in such a way as to reduce the number of uncertain parameters. In the extreme this would lead, for example, to the lake-scale, total phosphorus, mass-balance formulations exemplified by models reviewed by Rockhaw [1979]. In these models, parameter variance is limited to uncertainty in the phosphorus apparent settling velocity. Other variance sources derive from loading and hydraulic washout estimates. This general approach toward an aggregate representation will produce useful predictions with relatively low variance. This approach, however, is not always appropriate. Scavia and Chapra [1977] discuss the underlying similarities between simple mass-balance and more detailed ecosystem approaches and suggest that if one is interested in seasonal dynamics of phytoplankton species composition, dynamic availability of phosphorus for algal growth, or in fact, any specific aspect of the ecosystem other than lakewide averaged total phosphorus concentration, then a more disaggregated modeling approach is required.

If more detailed ecosystem models are required, there are other means to reduce parameter variance and subsequently model output variance. One way is through laboratory and field programs designed to study biological, chemical, and physical processes associated with the parameters. In this way, at least parts of the assumed stochastic variability in parameter values could be explained and simulated deterministically. Thus the remaining parameter uncertainty (or variance) would be reduced.

Another approach to reducing parameter variance is to limit the range of true state variables aggregated as a single model state variable and characterized by assumed constant parameters. For example, in the model examined herein, all phytoplankton are modeled as a single component characterized by a particular set of parameter values. Because the range of actual phytoplankton species being characterized is large, the variance associated with the parameters is large. If the phytoplankton were separated into functional groups, parameters characterizing each group would have lower variance. This procedure would obviously lead to more parameters and thus more variance sources; however, whether an increased number of sources, each with lower variance, will increase or decrease output variance is yet to be shown. Regardless of how parameter variance is to be reduced, one could not reduce the variance of each parameter consistently or simultaneously; anyway, it probably is not the most efficient approach.

Consequently, a correlation analysis was performed with the propagated covariance matrix to identify the most sensitive parameters. Each state variable was sensitive to different parameters at different times; however, some general patterns were observed. All of the state variables were correlated with KIC, the phytoplankton maximum growth rate, early in the year. This was because phytoplankton production was the dominant process at that time. After this initial time period, CTG and CCHL, two parameters related to grazing by herbivores, became important because the herbivores responded to increased concentration of phytoplankton during this time period. During the period of relative dynamic equilibrium in summer, the phosphorus/chlorophyll stoichiometric ratio, PCHL, emerged as the most important parameter for nutrient state variables. This was most likely because during relatively stable periods, stoichiometric parameters control partitioning of nutrients among various components of their cycles. From this analysis it appeared that state variables and variance associated with 'spring bloom' conditions were controlled most by variance in KIC and CTG, whereas those associated with summer conditions were controlled most by the stoichiometric ratios PCHL and CCHL. This suggests that model output variance could be reduced significantly by reducing the variances associated with these parameters. These reductions could be accomplished by the approaches discussed above.
Another approach to reducing variance that can often result in both lower variance and better model structure is through parameter estimation and model structure identification algorithms such as the Extended Kalman Filter [Kalman, 1960; Kalman and Bucy, 1961; Gelb, 1974]. For example, Koivo and Phillips [1976] and Bowles and Grenney [1978] used this algorithm to estimate parameter values in stream DO-BOD and water quality models. Beck [1976] and Beck and Young [1976] demonstrated use of the algorithm for identifying missing structure of DO-BOD models of rivers and subsequently reducing output variance. The Extended Kalman Filter as well as nonlinear least squares regression were applied to the model and data described herein [Scavia, 1980d]. In our application the utility of these approaches was constrained severely by the small data base relative to size of the problem, an outcome that should be expected because the algorithms generally require (1) high-density data, (2) low dimensionality of the problem, and (3) accurate models [Moore, 1978].

The present study focused on comparisons within a subset of potential variance sources. It is recommended that there be further investigations to explore variance caused by the 15 parameters that have been assumed to be known perfectly. Extension of the present analysis to all 22 parameters will be straightforward operationally. The difficulty will lie in estimating the additional parameter input variances. Some could be examined relatively easily because the literature is replete with their measurements (e.g., phytoplankton sinking rate); however, others may require further experimental study initially (e.g., carnivore grazing rate). An effort should also be made to quantify model equation errors independent of parameter variability. This could be accomplished by error analysis and identification of submodels in relation to the specific processes they describe. These problems will be more tractable for algorithms such as the Kalman Filter. Estimated errors in the submodels could be accumulated in the overall model easily because most processes are used simply in linear combinations to describe state variable dynamics.

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REFERENCES


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