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 Orlob*, 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., *Vallentyne and Thomas*, 1978]; yet quantitative limits of confidence are lacking for these models [*Mueller*, 1980], unlike many of their simpler counterparts [e.g., *Chapra and Reckhow*, 1979; *Reckhow*, 1979; *Lettenmaier 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 mod-

els 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*, 1979; *Gardner et al.*, 1980*b*; *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 Matystik*, 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* [1980*a*], *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]:

$$\dot{P} = AP + PA^T + Q \tag{1}$$

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

$$A_{ij} = \partial g_i / \partial x_j \tag{2}$$

where g_i is the model equation for the ith state variable and x_j is the jth 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* [1980*a*], 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.
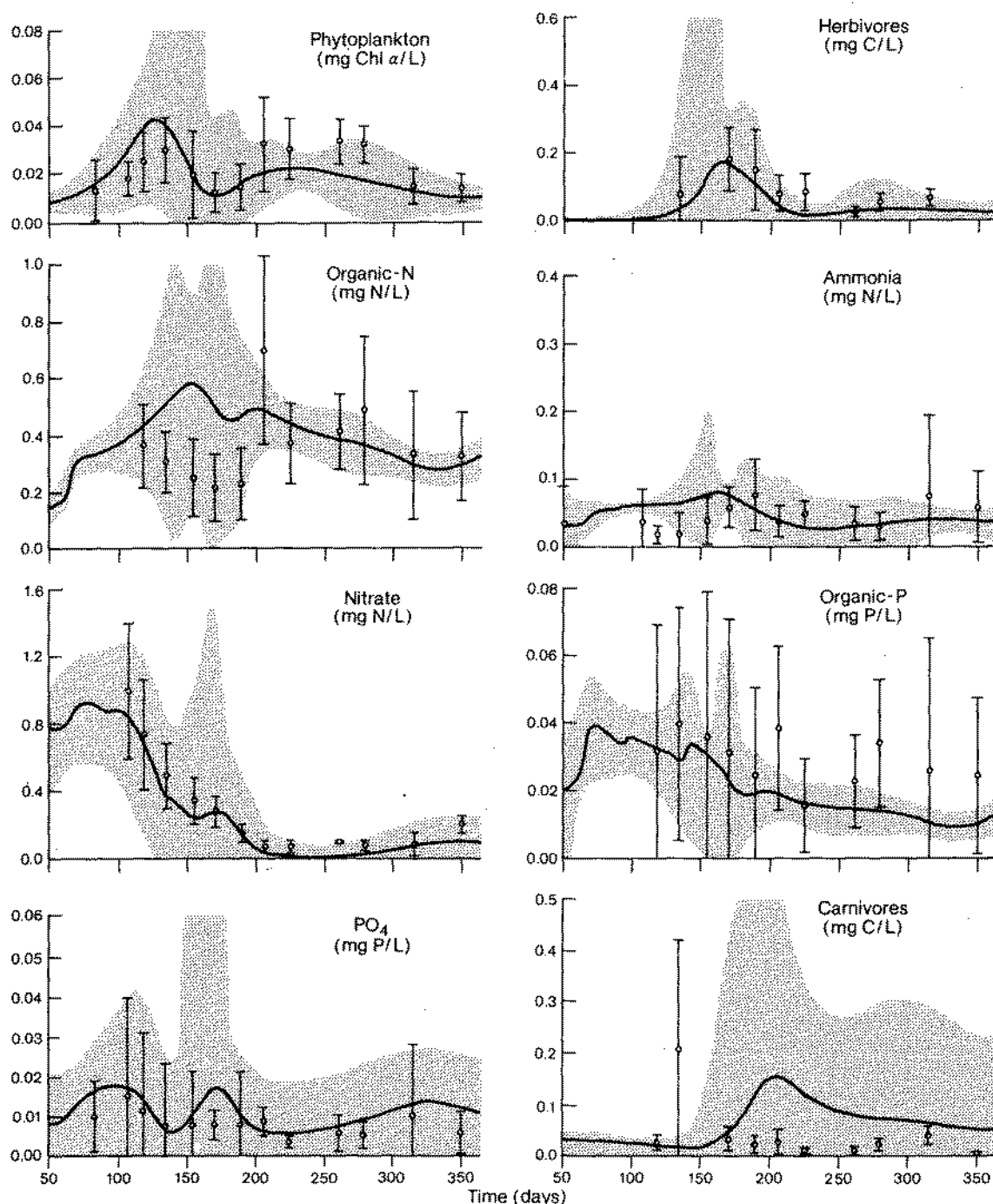
Fig. 1. Plots of eight state variable trajectories (smooth curve) from Saginaw Bay model. Model error estimates are represented as ±1 standard deviation bands (shaded) from first-order analysis. Data (circles with error bars) are represented as baywide mean plus or minus standard deviation of all samples.

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

TABLE 1. Statistics Used for State-Variable Initial Conditions

Variable	Mean	Variance	Coefficient of Variation, %
Phytoplankton	0.0092 mg Chl l^{-1}	2.98×10^{-5}	59
Herbivores	0.0075 mg C l^{-1}	2.0×10^{-5}	60
Organic N	0.14 mg N l^{-1}	3.8×10^{-3}	44
Ammonia	0.031 mg N l^{-1}	2.6×10^{-3}	164
Nitrate-nitrite	0.75 mg N l^{-1}	1.0×10^{-1}	42
Organic P	0.02 mg P l^{-1}	4.0×10^{-4}	100
PO$_4$	0.0084 mg P l^{-1}	1.44×10^{-4}	143
Carnivores	0.032 mg C l^{-1}	3.0×10^{-4}	54

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 variation of stratified (partitioned in time) samples because loading variability was much higher in the early part of the year. External loads enter model equations as simple bias terms: $\dot{x} = g(x, t) + L/V$, $L = $ load (g m^{-3} day^{-1}), and $V = $ volume (0.806 $\times$ 10^{10} 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.* [1978], *Zison 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 Matystik* [1980] considered mixing at the Saginaw Bay–Lake Huron interface. *Bierman and Dolan* [1976], *Bierman* [1976], and *Bierman et al.* [1980] considered mixing between inner and outer bay segments. Mixing characteristics and transport have also been examined for 5-segment [*Richardson and Bierman*, 1976], 16-segment [*Rich-*

ardson, 1976], and 33-segment [*Canale and Squire*, 1976] conceptualizations. In each case, mixing parameters were adjusted temporally until tracers (temperature, chloride) were simulated accurately. In the case of a two-segment bay, all transport is parameterized by the mixing parameter. For three or more segments, advective transport is specified and the mixing parameter used to refine tracer simulations. This procedure allows one to describe mixing empirically in a well-defined way, and thus uncertainty surrounding the mixing parameter should be quite low. In fact, mixing parameters from all of the above studies are similar in magnitude. Experience with calibration of the inner bay model to chloride concentrations indicated that once a calibration was achieved, changes in the mixing parameter had significant effects only for changes greater than approximately 10%. Others have had similar experience (D. M. DiToro, D. M. Dolan, personal communications, 1980). Although this is not an accurate estimate of its uncertainty, the variance of the mixing parameter was estimated from the parameter values and a CV of 10%.

Input variances used herein are generally larger than those used in similar Monte Carlo comparisons [*Scavia et al.*, this issue]. In that paper, input variances were calculated to correspond to variances of the values sampled from random number generators (given triangular distributions). Herein, the variances are calculated from actual values published in the literature.

RESULTS

From the model, input statistics, and variance propagation technique described above, state-variable variance estimates were made for an annual simulation based on variances of the initial conditions and given parameters. Resulting variances are represented as model output plus or minus its standard deviation in Figure 1 and are normalized as CV (standard deviation/state variable value) in Table 5.

Peaks in variance estimates occurred at times when the state variables were changing fastest. *Gardner et al.* [1980b] found this property to be common among several predator-prey models. Maximum CV (generally in late spring) ranged between 148 and 772%; however, the average CV during summer ranged between 33 and 407%. While these values are large, they are in many cases comparable to the variability within the bay itself (Table 5, Figure 1). *Gardner et al.* [1980b] also observed that summer is the most predictable period of

TABLE 2. Statistics for Volume Specific State-Variable Loads

Variable	Mean	Variance	Coefficient of Variation, %
Day 50–115			
Organic N	3.1×10^{-3}	2.3×10^{-5}	155
Ammonia	4.7×10^{-4}	2.6×10^{-7}	102
Nitrate-nitrite	8.2×10^{-3}	5.8×10^{-5}	93
Organic P	8.2×10^{-5}	1.0×10^{-6}	122
PO$_4$	1.6×10^{-4}	1.9×10^{-8}	87
Day 165–365			
Organic N	4.6×10^{-4}	7.8×10^{-8}	60
Ammonia	2.1×10^{-4}	1.1×10^{-8}	51
Nitrate-nitrite	2.7×10^{-4}	3.4×10^{-8}	68
Organic P	6.9×10^{-5}	1.2×10^{-8}	159
PO$_4$	9.4×10^{-5}	3.7×10^{-9}	65

Units are mg l^{-1} day^{-1}.

TABLE 3. Parameter Values Assumed Uncertain in Saginaw Bay Model

Parameter	Value	Unit	Definition
KIC	0.58	day^{-1}	maximum phytoplankton specific growth rate
KMP	0.005	mg P l^{-1}	Michaelis constant for phosphorus
CGT	0.06	l mg C^{-1} day^{-1} °C^{-1}	herbivorous zooplankton filter rate
CCHL	30.0	mg C mg Chl^{-1}	carbon to chlorophyll ratio
KMPL	0.02	mg l^{-1}	Michaelis constant for phytoplankton
K4T	0.006	(day °C)$^{-1}$	herbivore respiration rate
PCHL	0.6	mg P mg Chl^{-1}	Phosphorus to chlorophyll ratio

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). None of the *CV* increased more than 20% when loading variances were included. In fact, only ammonia-nitrogen (NH$_3$-N) and nitrate-nitrogen (NO$_3$-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 as-

TABLE 4. Statistics for Parameter Values

Variable	Mean	Variance	Coefficient of Variation	Number	Source	Comment
KIC	0.64	0.057	37	26	*Canale et al.* [1974]	
	0.48	0.059	48	51	*Canale and Vogel* [1974]	diatom
	0.43	0.068	43	48	*Canale and Vogel* [1974]	greens
	0.24	0.026	24	30	*Canale and Vogel* [1974]	flagellates
	0.48	0.109	48	47	*Canale and Vogel* [1974]	blue-greens
	0.46	0.079	46	202	*Canale and Vogel* [1974]	all species
	0.68	0.34	85		*Ford et al.* [1978]	
	0.34	0.011	29		*Ford et al.* [1978]	
	0.58	0.08	48			used in this study
KMPL	0.053	0.0075	163	14	*Scavia* [1980a]	*Bosmina, Diaptomus, Daphnia*
	0.022	0.00065	116	8	*Scavia* [1980a]	*Bosmina* only
	0.02	0.00027	82			used in this study
CGT	0.088	0.0063	90	34	*Zison et al.* [1978]	all species, all temperatures
	0.09	0.0043	72	17	*DiToro et al.* [1971]	assumed at 20°C
	0.016	0.0001	64	10	*Wetzel* [1975]	Cladocerans assumed at 20°C, 0.01 mg C individual^{-1}
	0.033	0.000157	38	4	*Wetzel* [1975]	Copepods assumed at 20°C, 0.004 mg C individual^{-1}
	0.025	0.0001	40	13	*Wetzel* [1975]	*Diaptomus gracilis*, 0.004 mg C individual^{-1}
	0.06	0.002	75			used in this study
K4T	0.012	4×10^{-5}	54	33	*DiToro et al.* [1971]	assume O$_2$: C = 2.75, maximum species
	0.013	4×10^{-5}	52	8	*DiToro et al.* [1971]	assume O$_2$: C = 2.75, all rates only
	0.023	3×10^{-4}	84	11	*Zison et al.* [1978]	maximum rates only
	0.016	6×10^{-5}	49	48	*Zison et al.* [1978]	all data
	0.006	2×10^{-5}	75			used in this study
CCHL	80	6400	100	42	*Jorgensen* [1979]	
	72	3241	80	32	*Canale et al.* [1974]	
	30	1000	105			used in this study
KMP	0.0075	3.7×10^{-5}	81	14	*Canale et al.* [1974]	
	0.006	4×10^{-5}	33		*Ford et al.* [1978]	
	0.003	1×10^{-6}	33		*Ford et al.* [1978]	
	0.005	6×10^{-6}	49			used in this study
PCHL	4.1	18.	104	27	*Jorgensen* [1979]	
	2.3	2.	60	23	*Canale et al.* [1974]	
	0.6	0.1	53			used in this study

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

Variable	Maximum	Summer Mean*	Observations†
Phytoplankton	593	78	52
Herbivores	772	206	65
Organic N	148	33	48
Ammonia	201	155	92
Nitrate-nitrite	550	407	40
Organic P	163	48	96
PO₄	552	186	115
Carnivores	707	266	67

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

sumed 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 $\approx 10^{10}$ m³) 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 NH_3-N and NO_3-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 true sensitivity (i.e., $\partial g_i/\partial x_j$) and parameter variance to determine important state variable-parameter pairs. *Gardner et al.* [1980a, 1981] caution and demonstrate that sensitivity analysis without consideration of parameter variance can 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 ($\rho = 0.81$), while phytoplankton and nitrate (NO₃) were less correlated ($\rho = 0.42$). 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 × 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

Variance Sources	Phyto-plankton	Herbivores	Organic N	NH₃	NO₃	Organic P	PO₄	Carnivores
Initial condition only	38	81	24	46	123	22	58	58
Parameters only	592	768	148	196	536	163	548	704
Parameters and initial conditions	593	772	148	201	550	163	552	707
Initial conditions and loads	38	81	25	55	148	26	60	59
Initial conditions, loads, and mixing parameter	38	81	25	55	151	26	61	60
Initial conditions, loads (×2), and mixing parameter	39	82	26	63	172	28	63	61
Initial conditions, loads (×10), and mixing parameter	41	84	33	106	291	45	81	69

TABLE 7. Correlation Coefficients Among State Variables and Parameters

	Day 141								Day 239							
	Phyto-plankton	Herbivore	Organic N	Ammonia	Nitrate	Organic P	PO₄	Carnivore	Phyto-plankton	Herbivore	Organic N	Ammonia	Nitrate	Organic P	PO₄	Carnivore
Phyto-plankton	1.0								1.0							
Herbivore	-0.96	1.0							-0.72	1.0						
Organic N	-0.82	0.92	1.0						-0.064	0.60	1.0					
Ammonia	-0.97	0.95	0.88	1.0					-0.72	0.50	-0.16	1.0				
Nitrate	-0.42	0.23	-0.13	0.32	1.0				-0.70	0.44	-0.23	1.0	1.0			
Organic P	-0.94	0.95	0.93	0.97	0.16	1.0			-0.58	0.58	0.11	0.84	0.81	1.0		
PO₄	-0.81	0.89	0.79	0.73	0.19	0.77	1.0		0.31	-0.04	0.48	-0.71	-0.74	-0.76	1.0	
Carnivore	-0.94	0.97	0.90	0.93	0.21	0.93	0.85	1.0	-0.30	-0.80	0.53	0.089	0.039	0.27	0.11	1.0
K1C	-0.14	0.11	0.32	0.31	-0.32	0.28	-0.27	0.14	0.38	-0.33	-0.057	-0.42	-0.40	-0.030	-0.22	-0.066
KMPL	-0.32	0.35	0.30	0.31	0.11	0.32	0.29	0.32	0.24	0.34	0.69	0.022	-0.033	0.34	0.091	0.34
CGT	-0.56	0.50	0.50	0.54	0.20	0.53	0.54	0.49	-0.70	0.75	0.59	0.16	0.11	0.30	0.14	0.53
K4T	0.23	-0.24	-0.19	-0.21	-0.084	-0.21	-0.22	-0.25	-0.064	-0.011	0.086	0.017	0.013	0.017	0.037	-0.26
CCHL	-0.69	0.74	0.60	0.64	0.24	0.64	0.63	0.71	-0.028	0.36	-0.019	-0.0035	-0.0088	0.037	-0.038	0.73
KMP	0.022	-0.032	-0.094	-0.066	0.12	-0.087	0.13	-0.038	-0.13	0.094	-0.022	0.17	0.17	-0.0075	0.082	0.010
PCHL	-0.17	-0.064	-0.32	0.12	0.71	0.061	-0.25	-0.049	-0.50	0.24	-0.36	0.86	0.87	0.89	0.94	-0.034

portant 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 ($| \rho | > 0.5$) in time and state-variable space. Some clear patterns emerge: (1) Early in the simulation, phytoplankton growth rate (K1C) 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 K1C, 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 those 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 those 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
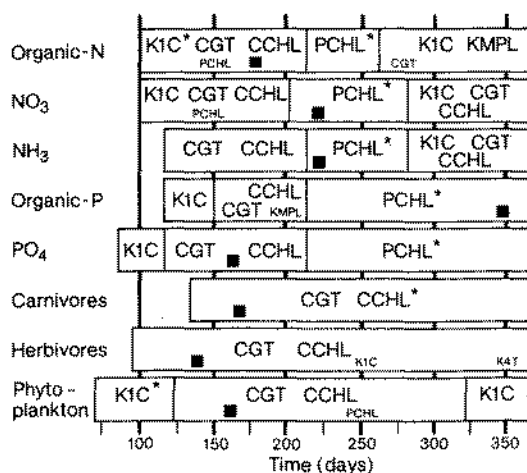
Fig. 2. Map of important parameters (defined in Table 3) for each state variable as a function of time. Solid squares represent time of occurrence of maximum coefficient of variation for each state variable. Parameter–state variable correlations greater than 0.8 are noted with asterisks. Large type represents important parameters during indicated intervals. Small type represents important parameters only at the time indicated.

summer model CV for all eight state variables ranged between 33 and 407%, whereas the annual average 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 NO_3-N (407%) 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 effected 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 *Reckhow* [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 K1C, 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, CGT 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 variances associated with 'spring bloom' conditions were controlled most by variance in K1C and CGT, 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*, 1980a]. 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 best 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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