

A SENSITIVITY AND ERROR ANALYSIS FRAMEWORK FOR LAKE EUTROPHICATION MODELING¹

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ABSTRACT: A framework for sensitivity and error analysis in mathematical modeling is described and demonstrated. The Lake Eutrophication Analysis Procedure (LEAP) consists of a series of linked models which predict lake water quality conditions as a function of watershed land use, hydrologic variables, and morphometric variables. Specification of input variables as distributions (means and standard errors) and use of first-order error analysis techniques permits estimation of output variable means, standard errors, and confidence ranges. Predicted distributions compare favorably with those estimated using Monte-Carlo simulation. The framework is demonstrated by applying it to data from Lake Morey, Vermont. While possible biases exist in the models calibrated for this application, prediction variances, attributed chiefly to model error, are comparable to the observed year-to-year variance in water quality, as measured by spring phosphorus concentration, hypolimnetic oxygen depletion rate, summer chlorophyll-a, and summer transparency in this lake. Use of the framework provides insight into important controlling factors and relationships and identifies the major sources of uncertainty in a given model application.

(KEY TERMS: eutrophication; modeling; sensitivity analysis; error analysis; simulation; water quality; lakes; watersheds; phosphorus; chlorophyll.)

INTRODUCTION

Scarcity of information is a problem which is typically encountered by agencies with responsibilities for managing lake water quality at a regional level. Many states have attempted to develop data bases for identifying problem conditions and prioritizing lakes for receipt of more intensive study and/or restoration. Intensive lake and watershed monitoring studies are rarely feasible in this context, owing to the large numbers of lakes which must be considered. Typically, available data may describe lake morphometry, watershed characteristics, and, in some cases, lake water quality, derived from limited monitoring. Hydrologic data may also be available, but rarely are direct nutrient loading measurements or results from intensive lake quality surveys. As a result, lake prioritization must be done without accurate water quality assessments and without complete understanding of the factors and relationships which control the water quality of each lake. Because of these data limitations, the problem assessments and rankings are subject to uncertainty.

Empirical models based upon data from a cross-section of lakes and/or watersheds may be used to estimate missing information. These include, for example, watershed land use/nutrient export relationships (Omernik, 1977), lake phosphorus retention models (Kirchner and Dillon, 1975), and lake phosphorus/chlorophyll models (Dillon and Rigler, 1974). Without direct nutrient loading measurements and intensive lake monitoring data, however, it is impossible to calibrate and test these models in each case. The range of models and coefficients available implies that choices must be made, often subjectively. Such decisions become easier and less subjective as regional experience with lake and watershed monitoring grows, as data bases are accumulated and analyzed, and as appropriate models are selected and regionally calibrated. Selection and use of these models introduces another element of uncertainty, particularly if a regional data base has not been established.

This paper describes and demonstrates a modeling framework which permits quantitative assessment of uncertainty in a useful and flexible way. The framework uses sensitivity and error analysis techniques to provide the user of a given model (or model linkage) with the following statistics for each predicted variable: (1) mean; (2) variance; (3) confidence limits; and (4) rankings of input variables with respect to (a) sensitivity, and (b) contribution to prediction variance. Use of the framework provides perspective on key assumptions and controlling factors in a given model application. Awareness of uncertainties and their dominant sources permits effective design of additional monitoring and/or modeling efforts and reduces the probability that a significant management decision will be made with undue confidence in the predicted outcome.

FRAMEWORK DESCRIPTION

The framework (Figure 1) is an extension and application of first-order error analysis procedures described previously (Benjamin and Cornell, 1970; Reckhow, 1977, 1979, 1980; Walker, 1977). A key aspect is the formulation of the sensitivity and error analysis procedures into a computer program

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from each of the input variables. This permits ranking of the input variables with respect to their impacts on the uncertainty in each response prediction. The uncertainty source ranking is perhaps more useful than the estimate of prediction error itself and is not strongly influenced by the approximations inherent in the first-order approach. The ranking can be used (1) for assessing the adequacy of input data for use with a given model (by comparing variance due to input uncertainty with variance due to corresponding model error); or (2) for setting priorities for further data collection and/or model development (by keying on variables or models which contribute the most uncertainty to the predictions).

The response standard errors reflect the combined influences of uncertainties in the input variables and model errors. Since all of the predicted variables in this application have minimum values of zero and have measurement and model error distributions which tend to be log-normal, the approximate 95 percent confidence limits (mean \pm 2 standard errors) of each response are calculated assuming a log-normal probability density function:

$$F_j = \exp(2\sqrt{\text{Var}(\hat{Y}_j) / \hat{Y}_j}) \quad (2)$$

$$\hat{Y}_j / F_j < Y_j < \hat{Y}_j F_j \quad (3)$$

where:

$$\hat{Y}_j = \text{predicted mean of variable } j.$$

As discussed above, these confidence limits are approximate in the case of a nonlinear model.

A by-product of the error analysis is a matrix of sensitivity coefficients:

$$S_{ij} = (d Y_j / d X_i) (X_i / Y_j) \quad (4)$$

A sensitivity coefficient can be interpreted as the percentage change in a given response variable induced by a 1 percent change in a given input variable. These coefficients are useful in a calibration procedure and provide insights into controlling factors and relationships in a given model application.

The framework described above has been coded in computer languages which are suitable for use on micro-computers, as well as time sharing systems (Walker, 1981). Model equations and variables are defined in a separate procedure which can be easily changed (to investigate alternative model formulations, for example) without modifying the main program, which handles data input, performs sensitivity and error analysis on each input and predicted variable, and generates output, while essentially treating the models as a black box (see Figure 1). Variable names and input values are provided in separate files. An interactive version permits the user to examine the consequences of modifying input and model error distributions. With the framework coded on a computer, the derivatives required for the sensitivity and error analysis can be estimated numerically using a finite-difference technique. This

eliminates the need for analytic differentiation of the models, which can lead to cumbersome expressions and increase the effort required to modify the model structure.

APPLICATION TO LAKE MOREY

Application of LEAP to a given lake requires the specification of a set of models and their respective error distributions, based upon regional data bases and regional modeling experience. The Appendix describes a set of models which has been selected in order to demonstrate the framework for Lake Morey, Vermont (Walker, 1980). Control pathways are depicted in Figure 2.

An attempt has been made to regionalize some of the models by using phosphorus/chlorophyll/transparency relationships derived from Vermont Lake data (Clarkson, 1979). While summer, epilimnetic phosphorus values may correlate better with summer chlorophyll-a or transparency (Carlson, 1977; Walker, 1979), spring values are used in this example because only spring phosphorus data were available for the Vermont lakes used to develop the regression models. The remaining lake models have been derived from northern temperate lake data (Walker, 1977, 1979). The watershed model, used for predicting average stream phosphorus levels from land use, is based upon a regression analysis of data from 116 watersheds in the northeastern U.S. (Meta Systems, 1978). The model linkage has been successfully tested on data from 30 Connecticut lakes for its ability to predict spring phosphorus levels based upon land use, water loading, and lake morphometry in lakes not impacted by point sources (Meta Systems, 1979). Tuning of the land use/nutrient export and phosphorus retention models to data from Vermont watersheds and lakes will enhance the regional applicability of the model structure and coefficients and is currently underway.

TABLE 1. LEAP Input Variables for Lake Morey.

Variable	Units	Mean	Standard Deviation
01 Forested Area	km ²	16.7	0.0
02 Agricultural Area	km ²	2.02	0.0
03 Urban/Residential Area	km ²	0.52	0.0
04 Forested P Conc.	mg/m ³	15	3.0
05 Agricultural P Conc.	mg/m ³	57	6.3
06 Urban/Residential P Conc.	mg/m ³	139	31.0
07 Lake Surface Area	km ²	2.05	0.0
08 Runoff Rate	m/yr	0.56	0.13
09 Atmospheric P Loading	mg/m ² -yr	30.0	10.0
10 Lake Mean Depth	m	8.2	0.0
11 Lake Maximum Depth	m	13.1	0.0
12 Thermocline Depth	m	9.0	0.0
13 Direct P Loading	kg/yr	75.0	25.0
14 Spring Oxygen Conc.	g/m ³	12.0	1.0
15 Watershed Model Error	-	1.0	0.30
16 P Retention Model Error	-	1.0	0.55
17 Mean Chlorophyll-a Model Error	-	1.0	0.37
18 Max. Chlorophyll-a Model Error	-	1.0	0.39
19 Secchi Depth Model Error	-	1.0	0.39
20 Oxygen Depletion Rate Model Error	-	1.0	0.23

The model framework used for demonstration purposes has a list of 20 input variables, which are given in Table 1 along with means and standard errors used in the Lake Morey analysis. LEAP output variables and predicted distributions are given in Table 2. Figure 3 indicates that variable distributions estimated using first-order analysis compare reasonably with distributions estimated using Monte-Carlo simulation (250 trials). Figure 4 compares the confidence ranges of five response variables with observed water quality data from Lake Morey for various years. Direct measurements of phosphorus loading are not currently available for comparison with the predicted loading distribution.

Figure 4 shows that the observed responses of spring phosphorus and chlorophyll-a generally lie in the upper half of the predicted confidence intervals. This suggests possible biases in the input variables or model framework, as applied to this lake. Two distinctive aspects of Lake Morey which may in part be responsible for this bias include the tendency for algal populations to concentrate in the metalimnion (influencing the chlorophyll/transparency relationship) and the potential importance of internal phosphorus recycling (Vermont Department of Water Resources, 1979). The lake has a thin hypolimnion (mean thickness 2.7 meters), which causes early oxygen depletion and pronounced buildup of phosphorus in the hypolimnion during the stratified season. The mass of total phosphorus recycled into the epilimnion at fall turnover in 1979 was roughly equivalent to the estimated annual average external loading (Walker, 1980). This potential for internal cycling may reduce the retention coefficient below the empirical prediction. Another possible source of bias is in the watershed model, which has been tested against data from only a few watersheds in Vermont (Meta Systems, 1978). Essentially all of the urban land use in the basin is clustered around the relatively steep lake shore and may contribute more runoff phosphorus than predicted by the watershed model. As shown in

Figure 4, the summer average mixed layer total phosphorus concentration in 1980 was about 15 mg/m^3 , more comparable to the LEAP mean prediction of 16.4 mg/m^3 than the observed spring values. More intensive lake and watershed monitoring is being done in 1981 in order to provide a basis for improving the model framework calibration.

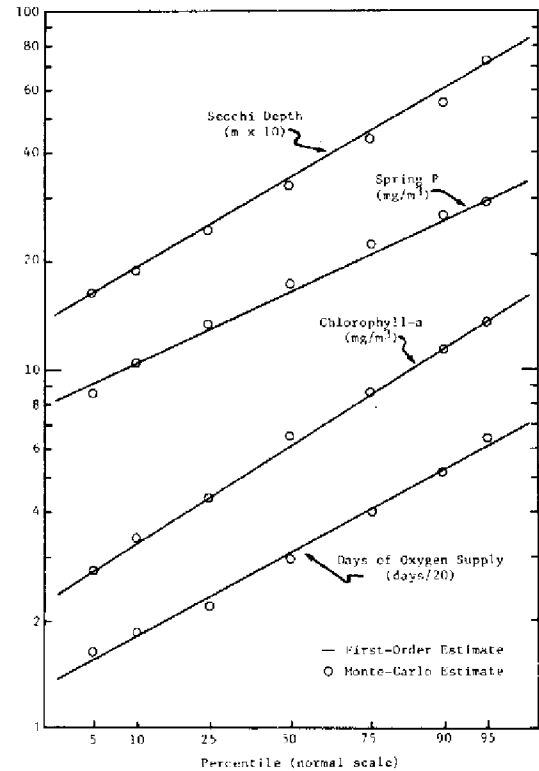
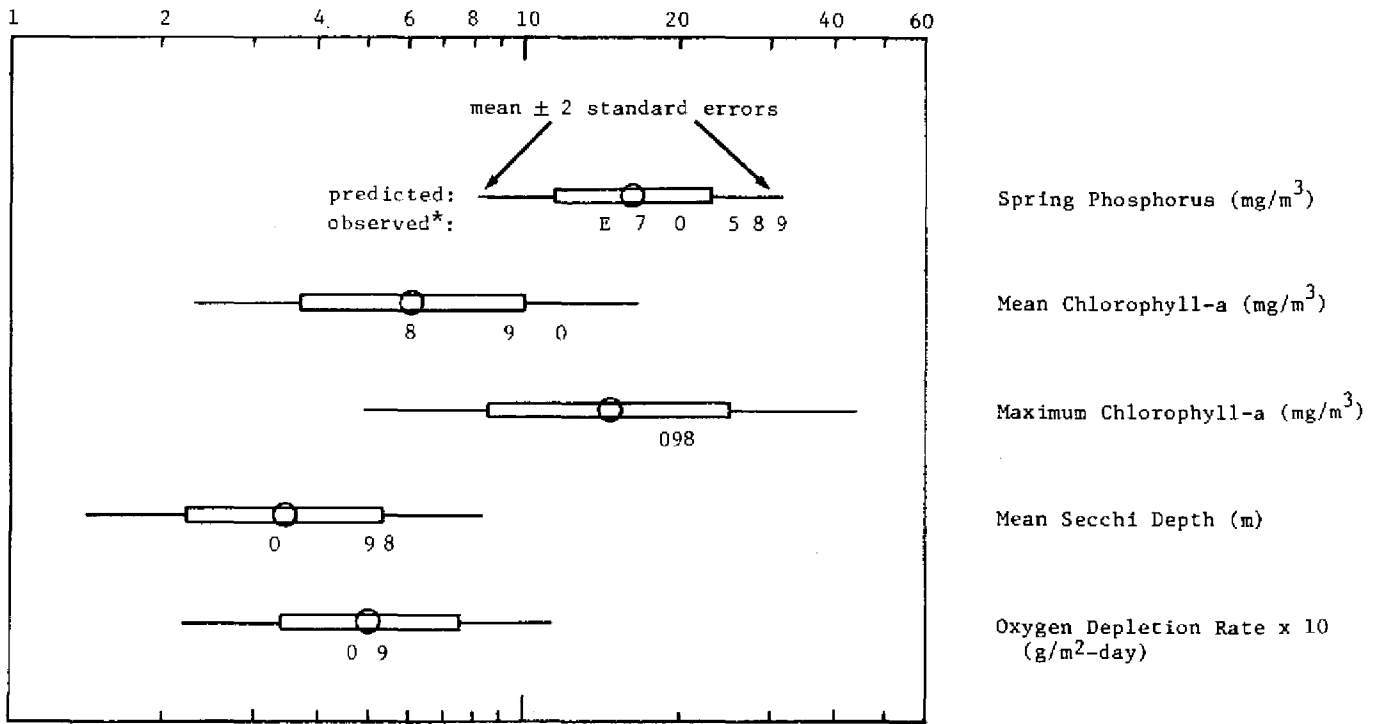


Figure 3. Estimated Output Variable Distributions Using First-Order Analysis and Monte-Carlo Simulation.

TABLE 2. LEAP Output Variables for Lake Morey.

Variable	Units	Mean	Standard Error	Confidence Range	
				2.5 Percent	97.5 Percent
01 Stream P Conc.	mg/m ³	22.8	7.4	11.9	43.6
02 Total P Loading	kg/yr	382	103	223	655
03 Surface Overflow Rate	m/yr	5.82	1.35	3.66	9.25
04 Hydraulic Residence Time	yr	1.41	0.31	0.91	2.19
05 1 - P Retention Coef.	-	0.51	0.14	0.30	0.87
06 Spring Phosphorus Conc.	mg/m ³	16.4	5.68	8.17	32.8
07 Mean Summer Chlorophyll-a	mg/m ³	6.07	2.93	2.31	16.0
08 Maximum Chlorophyll-a	mg/m ³	14.7	7.97	4.96	43.5
09 Mean Summer Secchi Depth	m	3.45	1.51	1.43	8.28
10 Hypo. 02 Depletion Rate	g/m ² -day	0.50	0.20	0.22	1.11
11 Mean Hypolimnion Depth	m	2.57	0.00	2.57	2.57
12 Days of Oxygen Supply	days	61.8	24.9	27.6	138
13 Phosphorus Residence Time	years	0.72	0.23	0.38	1.35
14 Trophic St. Discriminant Score	-	0.025	0.006	0.016	0.04
15 Eutrophic Probability	-	0.02	0.03	0.00*	0.18*
16 Mesotrophic Probability	-	0.75	0.19	0.32*	0.77*
17 Oligotrophic Probability	-	0.23	0.22	0.68*	0.05*

*Trophic state probability ranges based upon discriminant score range.



* symbol = last digit of sampling year (1975-80)

E = summer epilimnetic mean total P, 1980

Figure 4. Observed and Predicted Lake Response Distributions.

Despite the possible biases in the current framework calibration, the predicted variance estimates are comparable to the year-to-year variabilities in observed conditions. For example, the coefficient of variation of the estimated spring phosphorus levels is 0.35, as compared with an observed year-to-year coefficient of variation of 0.34, based upon 1977-80 data. The latter variations are attributed to natural causes, since no major changes in watershed land use or point source discharges are known to have occurred during this period. The timing of spring phosphorus sampling in relation to meteorologic and hydrologic variations which influence the characteristics of spring runoff probably contribute substantially to the observed year-to-year variations.

A matrix of sensitivity coefficients is given in Table 3. As discussed above, a sensitivity coefficient represents the expected percentage change in a given response variable for a 1 percent increase in a given input variable or model error term. For example, spring phosphorus concentration has a sensitivity coefficient of about 0.2 with respect to direct phosphorus loading, which, in this case, represents estimated septic tank and waste treatment lagoon inputs (VDWR, 1979). Thus, a 10 percent reduction in this input would be expected to result in a 2 percent reduction in spring phosphorus. This prediction is tentative, however, since the framework may not be correctly calibrated. The sensitivity of in-lake conditions to these direct inputs is a key management issue which will be

examined after refinements in the framework are made based upon additional watershed and lake sampling.

Table 4 identifies the sources of uncertainty in the prediction of each response as the percentage of total variance attributed to each input variable or model error term. Generally, the model error terms tend to dominate over input variable uncertainty. For example, despite the fact that direct phosphorus input is specified with a coefficient of variation of 0.33 (Table 1), it accounts for only 3.6 percent of the total variance in the prediction of spring phosphorus.

Since model error terms seem to be important, some discussion of their sources and significance is warranted. Model standard errors are generally estimated by comparing observations with predictions for a cross-section of lakes and/or watersheds. The gross standard error calculated in this way reflects the combined influences of measurement errors in the independent and dependent variables and true differences between the observed and predicted values. As discussed above, it is appropriate, where possible, to subtract measurement error variance from total error variance before using the variance estimate in the framework. Measurement error would include, for example, errors in estimates of average conditions based upon limited numbers of grab samples taken during a given season or year. The remaining error component reflects true year-to-year variations, as well as differences between the long-term-average predictions and responses. Current data sets not permit distinguishing between these two types of model

TABLE 3. Sensitivity Coefficient Matrix for Lake Morey.

Input Variable	Units	Predicted Variables					
		06 Spring P	07 Summer Chl-a	09 Summer Secchi	10 HOD	12 Days 02 Sup.	14 T.S. Score
01 Forested Area	km ²	-0.235	-0.211	-0.137	-0.221	0.224	-0.128
02 Agric. Area	km ²	0.095	0.085	-0.054	0.089	-0.089	0.108
03 Urban/Res. Area	km ²	0.087	0.078	-0.050	0.082	-0.081	0.090
04 Forested P Conc.	mg/m ³	0.368	0.329	-0.209	0.345	-0.340	0.367
05 Agric. P Conc.	mg/m ³	0.167	0.151	-0.097	0.159	-0.158	0.169
06 Urban/Res. P Conc.	mg/m ³	0.106	0.095	-0.061	0.100	-0.099	0.106
07 Lake Surface Area	km ²	-0.130	-0.116	0.075	-0.122	0.123	-0.252
08 Runoff Rate	m/yr	-0.130	-0.116	0.075	-0.122	0.123	0.007
09 Atmos. P Load	mg/m ² -yr	0.161	0.144	-0.092	0.152	-0.150	0.161
10 Lake Mean Depth	m	-0.215	-0.192	0.125	0.564	0.423	-0.176
11 Lake Maximum Depth	m	--	--	--	--	2.091	--
12 Thermocline Depth	m	--	--	--	--	-2.196	--
13 Direct P Loading	kg/yr	0.197	0.176	-0.112	0.185	-0.183	0.196
14 Spring Oxygen Conc.	g/m ³	--	--	--	--	1.000	--
15 Watershed Model Error	--	0.642	0.574	-0.361	0.604	-0.586	0.642
16 P Retention Model Error	--	-0.477	-0.428	0.281	-0.449	0.460	--
17 Chlorophyll-a Model Error	--	--	1.000	--	--	--	--
19 Secchi Depth Model Error	--	--	--	1.000	--	--	--
20 02 Depl. Rate Model Error	--	--	--	--	1.000	-0.952	--

TABLE 4. Variance Component Matrix for Lake Morey.*

Input Variable**	Units	Predicted Variables					
		06 Spring P	07 Summer Chl-a	09 Summer Secchi	10 HOD	12 Days 02 Sup.	14 T.S. Score
04 Forested P Conc.	mg/m ³	4.48*	1.85	0.91	2.99	2.84	10.67
05 Agric. P Conc.	mg/m ³	0.29	0.12	0.06	0.19	0.19	0.69
06 Urban/Res. P Conc.	mg/m ³	0.46	0.19	0.10	0.31	0.30	1.11
08 Runoff Rate	m/yr	0.75	0.31	0.16	0.50	0.50	0.01
09 Atmos. P Load	mg/m ² -yr	2.39	1.00	0.49	1.60	1.55	5.70
13 Direct P Loading	kg/yr	3.56	1.47	0.73	2.38	2.30	8.47
14 Spring Oxygen Conc.	g/m ³	--	--	--	--	4.28	--
15 Watershed Model Error	--	30.83	12.70	6.10	20.56	19.05	73.36
16 P Retention Model Error	--	57.22	23.72	12.36	38.29	39.40	--
17 Chlorophyll-a Model Error	--	--	58.65	--	--	--	--
19 Secchi Depth Model Error	--	--	--	79.11	--	--	--
20 02 Depl. Rate Model Error	--	--	--	--	33.17	29.59	--
Squared Coef. of Variation		0.12	0.23	0.19	0.16	0.16	0.08

*Percent of prediction variance attributed to given input variable or model error.

**Remaining input variables (Table 1) specified without error.

error. The data in Figure 4 reveal substantial year-to-year differences that cannot be explained on the basis of sampling or measurement error. For Lake Morey, monitoring data from more than one year are needed in order to provide adequate bases for assessing existing conditions or for calibrating a model framework.

CONCLUSIONS

The paper has described and demonstrated a framework which facilitates sensitivity and error analysis in a modeling

exercise. The framework provides insight into controlling factors and relationships and forces the user to be aware of prediction uncertainties and their sources. While demonstrated for a lake eutrophication modeling problem, the framework is of general applicability to many mathematical modeling problems encountered in water resources and other fields. The selection and the calibration of a model or set of models for use in a given problem are still key elements.

The needs for regional calibration and testing of the watershed and lake models used in the eutrophication model have been discussed and demonstrated. In the Lake Morey case,

prediction uncertainties attributed to watershed model error and lake model error tend to dominate over those attributed to input variable error. The variance in the predictions is, however, comparable to the year-to-year variance in lake water quality. This year-to-year variability may be a significant component of watershed and lake model errors. Analysis of data from a number of watershed/lake systems, each sampled more than one year, would provide insight into error sources and permit better interpretation of predictions derived from empirical lake models.

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Appendix

FUNCTIONS USED IN LEAP APPLICATION TO LAKE MOREY

Note:

X values refer to input and model error variables (Table 1).
Y values refer to output variables (Table 2)
LOG = natural (Base-e) logarithm.

Watershed Model for Stream P Concentration (Meta Systems, 1978):

$$AW = X(1) + X(2) + X(3)$$

$$Y(1) = X(15) [X(1) X(4) + X(2) X(5) + X(3) X(6)] / AW$$

Total Phosphorus Input (mass balance):

$$Y(2) = Y(1) AW X(8) + X(7) X(9) + X(13)$$

Surface Overflow Rate and Hydraulic Residence Time:

$$Y(3) = X(8) [AW + X(7)] / X(7)$$

$$Y(4) = X(10) / Y(3)$$

1 - Phosphorus Retention Coefficient (Walker, 1977):

$$Y(5) = 1 / (1 + .82 X(16) Y(4)^{.45})$$

Spring Phosphorus Concentration:

$$Y(6) = Y(5) Y(2) / [X(7) Y(3)]$$

Summer Mean Chlorophyll-a (Clarkson, 1979):

$$Y(7) = X(17) \text{EXP}[-.698 + .895 \text{LOG}(Y(6))]$$

Summer Maximum Chlorophyll-a (Clarkson, 1979):

$$Y(8) = X(18) \text{EXP}[-.354 + 1.088 \text{LOG}(Y(6))]$$

Summer Mean Secchi Depth (Clarkson, 1979):

$$Y(9) = X(19) \text{EXP}[2.847 - .576 \text{LOG}(Y(6))]$$

Hypolimnetic Oxygen Depletion Rate (Walker, 1979):

$$XI = -15.6 + 20.0 \text{ LOG}(Y(6))$$

$$LZ = \text{LOG}(X(10))$$

$$LH = -3.58 + .0204 XI + 1.98 LZ - .385 LZ^2$$

$$Y(10) = X(20) 10^{LH}$$

Mean Hypolimnion Depth (Walker, 1979):

$$Y(11) = X(10) [X(11) - X(12)] / X(11)$$

Days of Oxygen Supply at Spring Turnover (Walker, 1979):

$$Y(12) = X(14) Y(11) / Y(10)$$

Phosphorus Residence Time:

$$Y(13) = Y(4) Y(5)$$

Trophic State Discriminant Score (Walker, 1977):

$$PO = Y(2) / [(1 + .82 Y(4)^{.45}) X(3) X(7)]$$

$$Y(14) = .001 PO^{.82} (Y(2)/X(7))^{.18}$$

Trophic State Probabilities (Walker, 1977):

$$DT = - Y(14)^{-.25}$$

$$PE = \text{EXP}(-18.51 - 20.49 * DT)$$

$$PM = \text{EXP}(-36.77 - 29.33 * DT)$$

$$PO = \text{EXP}(-53.80 - 35.65 * DT)$$

$$PSUM = PE + PM + PO$$

$$Y(15) = PE/PSUM$$

$$Y(16) = PM/PSUM$$

$$Y(17) = PO/PSUM$$