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Documentation of CLEANX: a generalized model for simulating the open-water ecosystems of lakes*

FOREWORD

In the lead article in this issue, CLEAN, a generalized lake ecosystem model, was described by the 25 investigators in the Eastern Deciduous Forest Biome, U.S. International Biological Program, who were responsible for its formulation.¹ Because of the interest in this model, the team that implemented it as a user-oriented interactive package has consented to make the software available through one of the authors, Richard A. Park, or from SCS. The version described here is CLEANX; it is used to simulate the open-water (pelagic) portions of lakes, as described in the previous paper.

Don Scavia (above, left), who had primary responsibility for implementation of CLEANX, has a BS and an MS in environmental engineering; he is currently a research assistant in the Fresh Water Institute. Jay Bloomfield (above, right), who worked closely with Scavia in the implementation and was instrumental in developing the original program code for the overall CLEAN model, also has BS and MS degrees in environmental engineering and is currently completing his PhD (his dissertation research is on modeling the decomposition process). John Fisher has a BS in mathematics

and is in the graduate mathematics program at Rensselaer Polytechnic Institute. He and James Nagy, currently a programmer at National Computer Software Systems, worked closely with the rest of the team in programming the model. Richard Park is an Associate Professor of Geology at Rensselaer Polytechnic Institute and is Chief Mathematical Ecologist of the Fresh Water Institute; his dual role was to supervise the implementation of the model and to serve as liaison with the multidisciplinary group involved in its formulation.

SUMMARY

This paper outlines the software for an open-water version of CLEAN, an ecosystem model for lakes. The modular program structure is described, examples of driving variables are given, and the output (including values of several parameters) is shown. The program, with extensive annotations to facilitate adaptation by potential users, is available from author Richard A. Park or from SCS.

* Contribution No. 168 from the Eastern Deciduous Forest Biome, U.S. International Biological Program

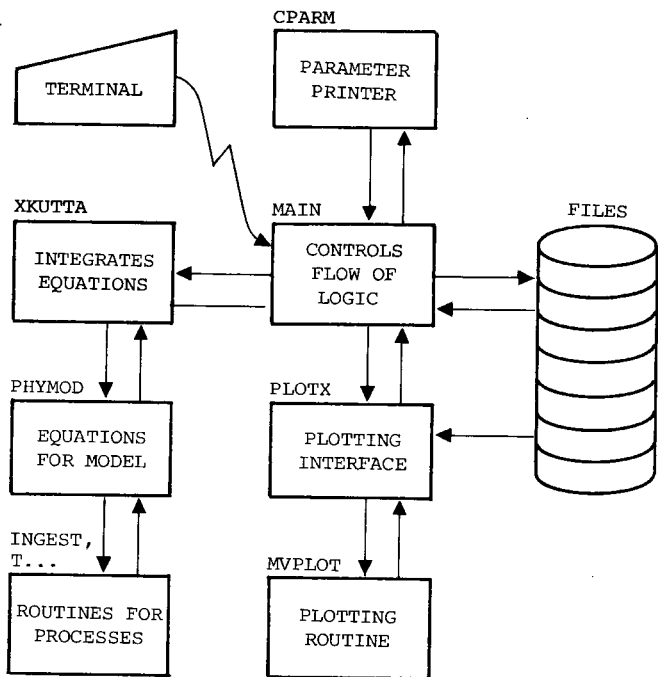


Figure 1 - Flow diagram of program logic

PROGRAM STRUCTURE

The model has been implemented in FORTRAN V on a UNIVAC 1108 as an interactive program. The program has a modular structure to increase computational efficiency and to permit addition of compartments and processes with minimal effort. The main routine is responsible for delegating control to integrating, plotting, and parameter-printing routines; also, it handles the editing of parameters, site constants, initial conditions, and perturbations, and it manipulates files (Figure 1).

Integration is performed by XKUTTA, a Runge-Kutta-Merson algorithm² modified to operate at a local relative error specified by the user. It is a fourth-order, variable-step method, carried out in extended precision. XKUTTA calls the subroutine PHYMOD, which evaluates the differential equations by extended-precision arithmetic manipulations. PHYMOD, in turn, calls additional subroutines and functions that define the process-level relationships and driving variables. After each interval in the simulation, control is returned to the main routine and the results are tabulated.

Upon completion of the integration, control can be passed to PLOTX, where control parameters which specify the plot format are set; plotting is initiated by the routine MV PLOT. Subsequently, control is passed back through the main routine to the user.

Other subroutines called by the main program at the user's discretion are for printing parameter values (CPARM) and saving edited parameter values (PRES). The main routine also prints initial conditions, messages that have been saved on a file, and a list of usable commands (Table 1).

The use of files is an integral part of this program. Parameter values are saved on file 9 and initial conditions are saved on file 10. During the execution of the program, temporary copies of these files are used for editing. Free-form editing is done using file 4. If the program is terminated by a *RES

Table 1
Program commands

Command	Options/Syntax	Description
*PRP, options	Parameter sections 1-9, A-E. No separators for a list.	Print parameters.
*PRI		Print initial conditions.
*RES		Save all changes made during cur- rent run (termi- nates program).
*END		Terminates pro- gram without saving changes.
*LAK, option	Lake Code: GEO, WIN default - GEO	Set driving variables for desired lake.
*MSG		Print all saved messages.
*EDP	Enter: $\text{\&EDIT param} =$ $xx \text{\&END}$	Edit a param- eter value.
*EDI	Enter: $\text{\&BEGIN param} =$ $yy \text{\&END}$	Edit an initial condition.
*HEL, option	B = brief listing default = extensive listing	List usable commands.
*READY		Check to see if program is ex- pecting input.
*PLT, <i>ab</i>	<i>a</i> : S - scaled log U - unscaled log (default) L - linear <i>b</i> : F - forced axis length C - constrain plot to maximum and minimum values of biomass as preset by user	Plot results of last integra- tion.
*INT		Integrate equations.
None	<i>Param</i> = <i>xx</i> where <i>Param</i> is any parameter, site constant, or initial condition (see Table 2)	Edit parameters and initial con- ditions in free- form format.

command, the temporary files are copied into the permanent files. Broadcast messages are saved on file 2, and a more detailed message listing is on file 3. Broadcast messages are displayed each time the program is executed; the detailed messages are obtained using a *MSG command (Table 1). The detailed list of commands is saved on file 11 and can be displayed by using a *HEL command. Unit 8 is used to store the integration data for subsequent plots and is retrieved by PLOTX.

DRIVING VARIABLES

Time-series of values of temperature and nitrogen are stored in the program in the form of equations utilizing Fourier series. Linearly interpolated values for other driving variables are returned from the routine CHART. Because of the application of this model to lakes of interest to the International Biological Program (IBP) and the Fresh Water Institute, data are included for Lake George in New York, Lake Wingra in Wisconsin, and Saratoga Lake in New York. The code also includes some data for Vorderer Finstertaler See, Austra, and Char Lake, Canada. However, only the data for Lake George have been checked for accuracy.

Data from Lake George were used in the example presented by Park and others¹ and in generating the output presented in this paper. Figure 2 shows the yearly variation of incident solar radiation, based on data corrected for ice cover and snow pack.³ The yearly pattern for water temperature (Figure 3) was derived from data averaged over the water column.³ The inputs of available phosphate and particulate and dissolved organic matter from streams and precipitation are shown in Figure 4.^{3,4} This version of the model is also driven by the nitrate-N and ammonia-N concentrations in the water column as shown in Figure 5.³ An important food source for the nonpiscivorous fish (perch, cisco, and bluegills) is bottom-dwelling insects; the insect submodel in CLEAN is not used in this pelagic version; rather, insect biomass is used as a driving variable (Figure 6).⁵

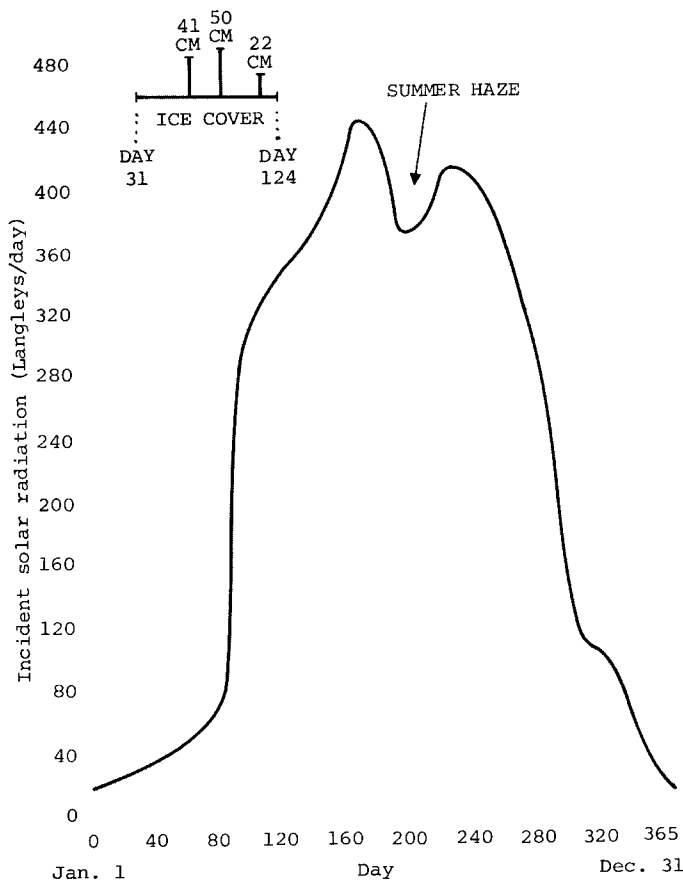


Figure 2 - Incident solar radiation, corrected for ice and snow pack

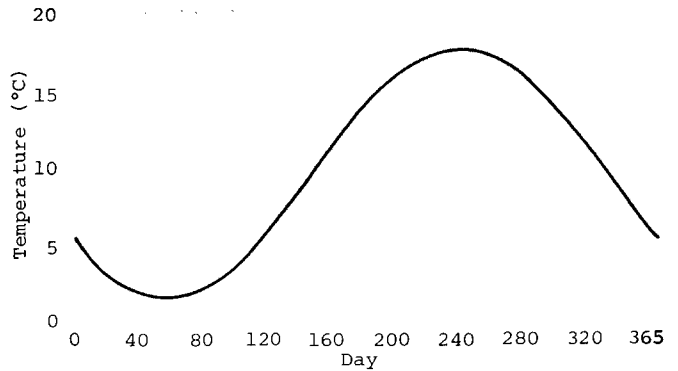


Figure 3 - Mean water-column temperature

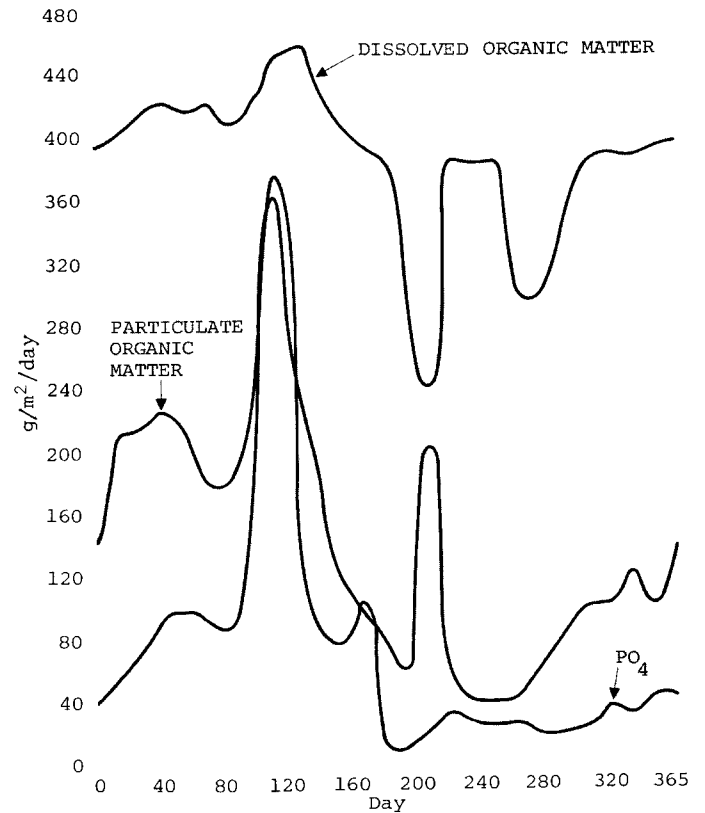


Figure 4 - Allochthonous inputs to Lake George

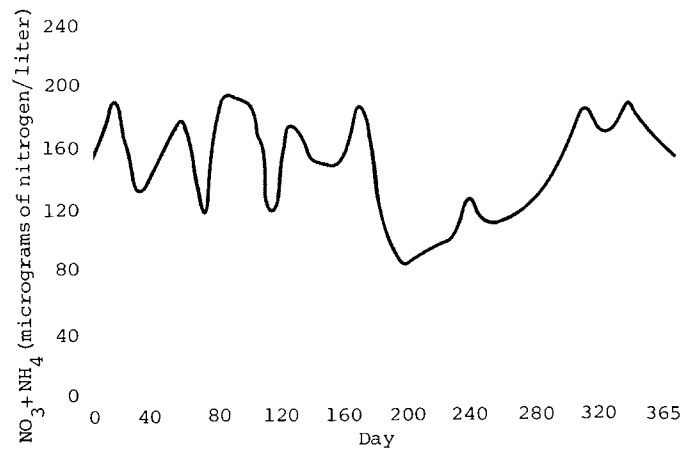


Figure 5 - Nitrate-N and ammonia-N concentration in Lake George

Table 2
Parameters and site constants

Name of variable in program	Name of variable in differential equation ¹	Units
ALPHA1	b	g/g/day
ALPHA2	a	g/g/day
BMIN	F_{min}	g/m ²
CMAX	C_{max}	g/g/day
CROWD	d	unitless
CROWDR	c	unitless
DEPTH	z	m
DOMMIN	DOM_{min}	g/m ²
E	f	unitless
EPS	e	1/m
HMAX	H_{max}	g/g/day
ISAT	I_s	ln/day
KBEH	$a_{j,n}$	unitless
KCAP	K_j	g/m ²
KDIF	K_{dif}	g/g/day
KDMORT	$K_{d,m}$	unitless
KDOM	K_{DOM}	g/m ²
KEXCR	U	1/day
KFISH	Z_f	1/day
KGON	$Z_{g,g}$	g/g/day
KMORT	Z_m	g/g/day
KN	N	g/m ³
KPMORT	$K_{p,m}$	unitless
KPOM	K_{pom}	g/m ²
KPOP	$b_{j,n}$	unitless
KO2	K_{r,O_2}	unitless
KP04	N	g/m ³
KRESP	K	unitless
KSED	K_{sed}	m/°C
KSV	K_{sv}	
KTEMP	$*$	°C ⁻¹
KU	U_j	unitless
OFMAX	$*$	°C
O2MIN	$O_{2,min}$	g/m ²
PHOPT	pH_{opt}	pH units
PHYTEX	K_2	m ² /g
PMAX	P_{max}	g/g/m ²
PSI	ψ	g/g/day
Q	Q	g/m ²
Q10	S_Q	e ^{°C⁻¹}
R	r	unitless
RMAX	R_{max}	g/g/day
SIGMA	σ	pH units
TCRIT	$*$	°C
TMAX	T_{max}	°C
TOPT	T_{opt}	°C
TREF	$*$	°C
TSPAWN	$C_{f,g}$	°C
TSTOP	$C_{f,g}$	°C
URES	K_{resp}	unitless
VMAX	V_{max}	g/g/day
W	w	unitless

* Parameters used for acclimation to temperature, not used in Reference 1.

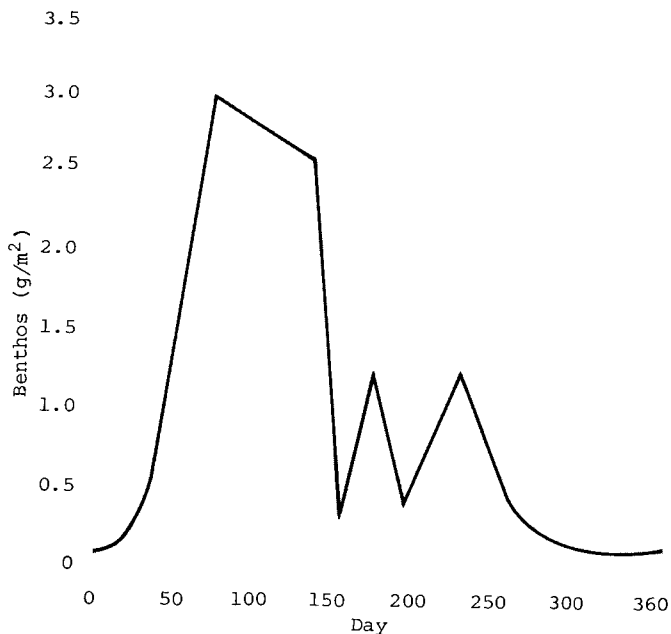


Figure 6 - Benthic insect biomass in Lake George

Table 3
Subscript definitions for parameters

Ecosystem Compartments

1. Nannophytoplankton
2. Net phytoplankton
3. Cladocerans
4. Copepods
5. Omnivorous zooplankton
6. Nonpiscivorous fish
7. Benthic insects
8. Piscivorous fish
9. Particulate organic matter
10. Dissolved organic matter
11. Decomposers
12. Phosphate

Process

1. Primary production, consumption, decomposer uptake
2. Decomposer hydrolysis
3. Respiration
4. Mortality
5. Gamete loss, decomposer excretion
6. Gamete loss
7. Fishing stress

```

***** PELAGIC MODEL (CLEANX) *****
DATE: 030674 (MMDDYY) TIME: 000609 (HHMMSS)

FWI TIME/SHARE MODELS (SUNYAR)

LAST UPDATE 3/4/74

FOR PERTURB. DO A *MSG.

READY
*MSG
NEW MSGS

3/4/74 THE FOLLOWING PARAMS ALLOW CHANGES IN THE
DRIVING FUNCTIONS:
KPOP(7,1) L. GEORGE PD4IN
KPOP(7,2) L. WINGRA PD4IN
KPOP(7,3) L. GEORGE TEMP.
KPOP(7,4) L. WINGRA TEMP.
FORM: PD4IN=KPOP( )>>(EXISTING FUNCTION)
TEMP.=KPOP( )>>(EXISTING FUNCTION)

2/21/74 MVPLLOT CHANGE: THE FOPMAT FOR THE X-AXIS IS
IS NOW DYNAMICALLY SELECTED TO AVOID THE
THE ***** PROBLEM FOR FIVE YEAR SIMULATIONS.
SOURCE IS NAMED 'MVPLLOTX'. OLD SOURCE IS
STILL 'MVPLLOT'. JSF

2/20/74 THERE ARE NEW PARAM VALUES IN THE PELAGIC MODEL...
A COPY OF YOUR VALUES IS ON MY DESK.

1/ 9/74 KUTTA NOW DEBUGGED...JAY

1/ 9/74 DEFAULT FOR LAKE CODE IS NOW LAKE GEORGE.

12/26/73 THE *PRP COMMAND NOW TAKES UP TO 6 OPTIONS:
FOR EXAMPLE *PRP,IA45
*PRP,I GIVES INITIAL CONDITIONS
*PRP GIVES ALL SECTIONS (EXCEPT INITIAL CONDITIONS)

12/26/73 THE *LAK COMMAND NOW TAKES AN OPTION:
FOR EXAMPLE *LAK,6 IS LAKE GEORGE.

12/26/73 A NEW VERSION OF KUTTA IS UP UTILIZING
RELATIVE LOCAL ERROR. ACCURC=.01 NOW
REPRESENTS A 1% LOCAL ERROR. CHECK RESULTS
CAREFULLY. IT'S NOT DEBUGGED.

12/13/73 USE ADD SOURCE.DIAG AFTER A 'FOR' TO SEE DIAGNOSTICS.

12/13/73 BENFISH, CLEANX AND MACRO ALL UP.

12/13/73 CLEANX NOW HAS ALL COMPARTMENTS DYNAMIC FOR PELAGIC
MODEL EXCEPT N03-NH4.

READY

```

Figure 7 - Model output - broadcast and detailed messages

```

KPOP(7,1)=.5
READY
LAST=365
READY
*INT
DATE: 030674 (MMDDYY) TIME: 001126 (HHMMSS) LAKE: GEO
-----
TIME  NAN  NET  CLAD  COPE  DMN1Z  NON-P  PISC  PD4  PDM  DOM  DEC
-----
1     .64  .30  .12  .30  .19  .30  .10  .129  1.50  100.00  .020
15    .64  .40  .12  .30  .17  .25  .10  .130  .89  102.78  .031
29    .65  .54  .11  .30  .16  .21  .09  .131  .63  105.16  .056
43    .69  .73  .11  .29  .15  .18  .09  .133  .54  109.90  .119
57    .73  1.01  .11  .29  .14  .16  .09  .135  .47  113.17  .105
71    .79  1.40  .11  .30  .14  .14  .08  .141  .35  114.76  .193
85    .90  2.09  .12  .32  .13  .12  .08  .155  .25  110.67  2.648
99    1.23  3.74  .14  .39  .14  .10  .08  .171  .33  98.37  4.293
113   1.84  6.88  .20  .55  .16  .09  .07  .162  .77  90.59  2.658
127   2.67  12.19  .36  .94  .18  .03  .07  .121  1.55  91.82  1.211
141   3.08  16.16  .87  2.06  .27  .07  .06  .057  3.54  96.29  .818
155   1.30  9.21  2.17  4.05  .71  .08  .06  .024  6.38  100.70  .864
169   .68  2.05  2.48  1.99  2.45  .14  .05  .026  5.66  103.03  .935
183   1.01  1.01  .80  .54  3.54  .26  .05  .031  2.85  101.40  1.045
197   1.43  .79  .57  .54  3.27  .92  .05  .026  1.92  97.88  .789
211   1.61  .62  .56  .55  2.50  .90  .05  .016  1.97  95.27  .593
225   1.26  .47  .56  .56  1.63  1.19  .06  .008  1.79  94.03  .506
239   .89  .34  .53  .54  1.02  1.19  .03  .005  1.29  93.44  .443
253   .71  .23  .50  .52  .71  .98  .10  .004  .88  93.03  .352
267   .64  .16  .47  .50  .56  .72  .12  .004  .62  92.60  .268
281   .60  .11  .42  .47  .48  .50  .13  .004  .48  92.17  .188
295   .57  .08  .38  .43  .42  .35  .13  .003  .40  92.31  .130
309   .56  .06  .34  .40  .37  .26  .12  .004  .34  93.07  .098
-----
MAX TIME. STEP= 14.0000 MAX ERR= .02%

323   .56  .04  .31  .37  .33  .19  .11  .005  .30  94.39  .087
337   .57  .03  .29  .35  .29  .15  .11  .006  .27  95.94  .092
351   .57  .03  .27  .33  .27  .12  .10  .007  .24  97.57  .112
365   .56  .03  .26  .31  .25  .10  .09  .009  .21  99.37  .150
-----
READY

```

Figure 9 - Model output - free-form editing and integration (time is in days, biomass is in grams per m² column of water, and available phosphate concentration is in grams per m³)

```

*PRP
DEPTH= 20.0 EPS= .2 PHYTEM= .1

*SPECIES*
*PARAM* (1) (2) (3) (4) (5) (6) (7) (8)
PMAX= 2.20 2.00 CMAX= 1.00 1.30 1.60 1.50 .00 1.00
ALPHA1= .0500 .0500 Q= .2 .2 .2 .5 .0 .5
ALPHA2= .0010 .0010 R= .0 .0 .0 .0 .0 .0
KN= 10.00 50.00 CROWDP= .10 .10 .10 .10 .10 .10
KPD4= .01 .15 KEXCR= .05 .01 .01 .01 .00 .01
ISAT= 550.00 350.00 KMORT= .001 .001 .002 .005 .000 .001
KRESP= .01 .01 PMAX= .01 .01 .01 .01 .00 .01
KPMORT= .70 .70 KCAF= 50.0 50.0 20.0 5.0 .0 5.0
KDMORT= .30 .30 CROWD= .010 .010 .010 .001 .000 .001
TCRIT= 40.0 40.0 40.0 40.0 .0 40.0
KPMORT= .50 .50 .50 .50 .40 .00 .40
KDMORT= .50 .50 .50 .40 .00 .40

(SPECIES,PROCESS)
*PARAM* 1.1 2.1 3.1 4.1 5.1 6.1 7.1 8.1 1.3 2.3 3.3 4.3 5.3 6.3 7.3 8.3
KTEMP= 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
DFMAX= 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
TREF= 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
TDPT= 28. 22. 22. 22. 22. 20. 20. 20. 28. 22. 22. 22. 22. 22. 20. 20.
TMAX= 35. 35. 35. 35. 35. 35. 35. 35. 35. 35. 35. 35. 35. 35. 35. 35.
Q10= 2.5 2.0 2.2 2.2 2.2 2.2 2.2 2.2 2.5 2.0 2.2 2.2 2.2 2.2 2.2 2.2

TSPAWN= 18.0 18.0 TSTOP= 21.0 21.0
KGNON= .001 .010 KFISH= .000 .100

W(I,J) (J) (I,J)
(1) (3) (4) (5) (6) (7) (8) (5) (6) (7) (6,8) (7,6)
(I) (2) (3) (4) (5) (6) (7) (8) (5) (6) (7) (8)
(9) (1) (2) (3) (4) (5) (6) (7) (8)
(11) (1) (2) (3) (4) (5) (6) (7) (8)

E(I,J) (J) (I,J)
(1) (3) (4) (5) (6) (7) (8) (5) (6) (7) (6,8) (7,6)
(I) (2) (3) (4) (5) (6) (7) (8) (5) (6) (7) (8)
(9) (1) (2) (3) (4) (5) (6) (7) (8)
(11) (1) (2) (3) (4) (5) (6) (7) (8)

BMIN(I,J) (J) (I,J)
(1) (3) (4) (5) (6) (7) (8) (5) (6) (7) (6,8) (7,6)
(I) (2) (3) (4) (5) (6) (7) (8) (5) (6) (7) (8)
(9) (1) (2) (3) (4) (5) (6) (7) (8)
(11) (1) (2) (3) (4) (5) (6) (7) (8)

KPOP(J,PROCESS) (PROCESS)
(1) (2) (3) (4) (5) (6) (7)
(3) (1) (2) (3) (4) (5) (6) (7)
(4) (1) (2) (3) (4) (5) (6) (7)
(I) (5) (1) (2) (3) (4) (5) (6) (7)
(6) (1) (2) (3) (4) (5) (6) (7)
(7) (1) (2) (3) (4) (5) (6) (7)
(8) (1) (2) (3) (4) (5) (6) (7)

--- PERTURBATION PARAMS

KBEN(J,PROCESS) (PROCESS)
(1) (2) (3) (4) (5)
(3) (1) (2) (3) (4) (5)
(4) (1) (2) (3) (4) (5)
(I) (5) (1) (2) (3) (4) (5)
(6) (1) (2) (3) (4) (5)
(7) (1) (2) (3) (4) (5)
(8) (1) (2) (3) (4) (5)

**DECOMPOSER PARAMS**
(1) (2) (3) (4) (5)
TOPT= 15. 14. 15. 21. 17.
TMAX= 35. 35. 35. 35. 35.
Q10= 2.2 2.2 2.2 2.2 2.2
KTEMP= 0. 0. 0. 0. 0.
DFMAX= 0. 0. 0. 0. 0.
TREF= 0. 0. 0. 0. 0.
KD2= 0. 0. 0. 0. 0.

(SPECIES 11)
VMAX= 5.0000 KMORT= .0100 KSED= .8000
KDOM=300.0000 PHOPT= .0000 KPCM= 50.0000
RMAX= .4500 SIGMA= .0000 KMORT= .5000
HMAX= 4.0000 KPMORT= .5000 KSV= 1.0000
PSI= .0500 DOMMIN= 60.0000

KBDF(10)= .0000 KSED(9)= .8000 PSI(9)= .0500
KUC(1)= .0700 KUC(2)= .0050 KUC(3)= .0050

READY
*PRI
BIC= .64 .30 .12 .30 .18 .30 10.00 .10 1.50 100.00
.02 .13
TFIRST= 1.00 LAST=365.00 STEP=14.0000 ACCURC= .500-002 IMAX= 9
READY

```

Figure 8 - Model output - parameter and initial-condition list (as given in Table 2)

PROGRAM OUTPUT

Upon execution, the model prints all broadcast messages and passes control to the user. The first command used, *MSG, is to print out all messages inserted by previous users (Figure 7). This allows colleagues to keep one another informed of recent changes. The parameters and initial conditions are printed using *PRP and *PRI (Figure 8). (Parameter names and subscript definitions are given in Tables 2 and 3.) As shown in Figure 9, a perturbation parameter (in this example, phosphate loading for Lake

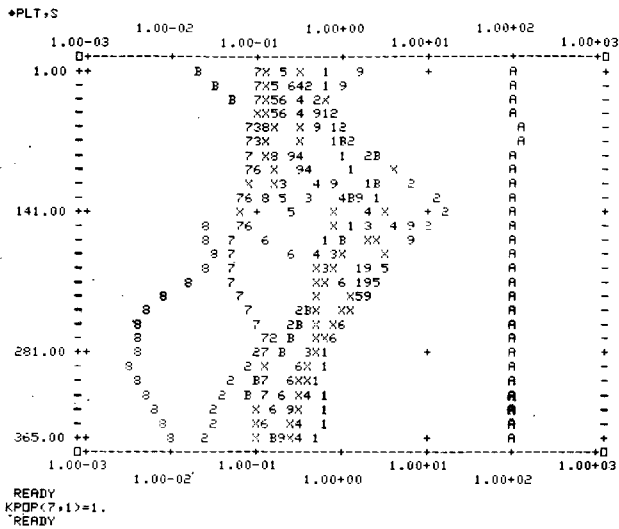


Figure 10 - Model output - plotting. Vertical axis represents time in days (beginning with January 1 and ending with December 31 in this example); horizontal axis represents biomass, expressed as grams per m² column of water. 1 = nannophytoplankton, 2 = net phytoplankton, 3 = herbivorous cladocerans, 4 = herbivorous copepods, 5 = omnivorous zooplankton, 6 = nonpiscivorous fish, 7 = piscivorous fish, 8 = available phosphate (in grams per m³), 9 = particulate organic matter, A = dissolved organic matter, B = decomposers.

George) is changed using the free-format editing feature, and an initial condition (TLAST) is changed. Also shown in Figure 9 are the tabulated results of an integration following the command *INT; the results are given for the user-specified interval (STEP) of fourteen days. The state variables, corresponding to those given by Park and others,¹ are nannophytoplankton, net phytoplankton, herbivorous cladocerans and copepods, omnivorous zooplankton, nonpiscivorous fish (including perch, cisco, and bluegills), piscivorous fish (including lake trout and bass), available phosphate, particulate organic

matter, dissolved organic matter, and decomposers. Because of the time required for the simulation, the user is given the option to abort the integration (using the command KILL) after twenty-five seconds of central processing unit (CPU) usage have elapsed (at "MAX. TIME"). In this example a 'carriage return' is used to continue the integration. Upon completion of the integration the plotting routine is called with the scaled plot option (*PLT,S) as shown in Figure 10. The compartments, numbered in the order in which they are displayed in the tabulation, are then plotted versus day of the year. After the plot, the perturbation parameter is reset.

ACKNOWLEDGEMENT

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REFERENCES

- 1 PARK, R.A. *et al.*
A Generalized Model for Simulating Lake Ecosystems SIMULATION August 1974 pp. 33-50
- 2 HAMMERLING, F.D.
Kutta
In Westly, G.W., J.A. Watts, eds., *The Computing Technology Center Numerical Analysis Library*, Union Carbide Corporation, Oak Ridge, Tennessee, 1971
- 3 WILLIAMS, S.L. CLESCERI, N.L., eds.
Diatom Population Changes in Lake George, New York Final report OWRR contract 14-31-0001-3387 1972
- 4 FUHS, G.W.
The Chemistry of Streams Tributary to Lake George, New York
Environmental Health Report #1
New York State Department of Health 1972
- 5 HENNINGSON, J.C.
A Study of the Benthic Macroinvertebrates in Selected Bays of Lake George, New York
MS thesis Rensselaer Polytechnic Institute Troy, New York 1973

EIGHTH ANNUAL SIMULATION SYMPOSIUM

Place: Tampa, Florida Date: March 12-14, 1975 Sponsor: SCS

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