

# Computer Programs for Calculating *In Situ* Phytoplankton Photosynthesis

E.J. Fee

Central and Arctic Region Department of Fisheries and Oceans Winnipeg, Manitoba R3T 2N6

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E.J. Fee

Central and Arctic Region
Department of Fisheries and Oceans
Winnipeg, Manitoba R3T 2N6

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### Table of Contents

		Page
Abs	,	ésumé
1	Prefac	e
2	Introd	uction
	2.1	Scope of the programs
	2.2	System requirements
	2.3	Time requirements
	2.4	Availability and transportability
3	Theor	y of the programs
	3.1	Simulation of photosynthesis vs depth curves
	3.2	Constants
	3.3	Interpolation procedures
	3.4	Integration method
	3.5	Calculation of cloudless solar PAR
	3.6	FITSOLAR
	3.7	PSPARMS
	3.8	YPHOTO and DPHOTO 8
	3.9	YTOTAL and DTOTAL
4	Using	the Programs
	4.1	Disk files
	4.2	Error Handling
	4.3	Data Used by More than one Program
		4.3.1 Solar data
		4.3.2 PAR extinction, $P_m^B$ , $\alpha^B$ , and chlorophyll data
		4.3.3 Hypsographic (lake area vs depth) data
		4.3.4 Mixing depth data
	-	4.3.5 Organization of data in DAT files
	4.4	Starting the Programs
	4.5	FITSOLAR
	4.6	PSPARMS
	4.7	YРНОТО
	4.8	YTOTAL
	4.9	DPHOTO
	4.10	DTOTAL
	4.11	Breakpointing Runs
	4.11	Run-time commands
	4.12 $4.13$	
5 3		wledgments
,	veiete	ences
_		List of Tables
le		Page
1		ata used in the programs
2		XTensions used in the programs
3		ary of input and output file EXTensions used by the programs
4	Defini	tions of mathemathical symbols

### List of Figures

Figure		Page
1	The procedure used to estimate in situ photosynthesis	. 22
2	The photosynthesis vs PAR curve, illustrating terminology	. 23
3	Example output from the program PSPARMS	. 23
4	Example cloudless solar PAR data generated by YPHOTO	. 24
5	Example output from the program YPHOTO	. 25
6	Example output from the program YTOTAL	. 26
7	Example output from the program DPHOTO	
8 .	Example output from the program DTOTAL	. 27

### Abstract

FEE, E.J. 1990. Computer programs for calculating in situ phytoplankton photosynthesis. Can. Tech. Rep. Fish. Aquat. Sci. 1740: v + 27 p.

This report describes computer programs for estimating in situ phytoplankton photosynthesis. The programs are written in Turbo Pascal and run on IBM compatible personal computers controlled by the DOS operating system. The theory of the programs is presented in detail along with instructions for use. Example data sets and resulting output are shown for each of the programs.

**Key words:** Limnology; oceanography; trophic dynamics; computer; primary production; model; simulation

### Résumé

FEE, E.J. 1990. Computer programs for calculating in situ phytoplankton photosynthesis. Can. Tech. Rep. Fish. Aquat. Sci. 1740: v + 27 p.

Ce rapport décrit des programmes d'ordinateur permettant d'évaluer in situ la photosynthèse du phytoplancton. Les programmes fonctionnent sur des ordinateurs individuels à système d'exploitation MS-DOS. Ils sont rédigés en Turbo PASCAL. Le rapport présente en détail la théorie des programmes ainsi que leur mode d'utilisation. Il présente des exemples de fichiers et le résultat final de chacun des programmes.

Mots-clés: Limnologie; océanographie; dynamique trophique; ordinateur; production primaire; modèle

### 1 Preface

This manual is a revision of the "primary production model" user's manual (Fee 1984), which is now out of print. This section is intended for readers familiar with the previous report; it describes how those programs have been changed. Users unfamiliar with the previous report should skip to the Introduction.

There have been several changes in terminology. The term "primary production" is no longer used to describe what these programs estimate. Primary production and primary productivity are terms that originate in trophic dynamic theory (Lindeman 1942): Primary production is the chemical energy in an ecosystem that is the direct product of photosynthesis, and primary productivity is the sum of all photosynthetic rates in an ecosystem. Because phytoplankton are the only important photosynthesizers in deep lakes and the offshore oceans, it is reasonable to argue that phytoplankton photosynthesis and primary production are the same thing in these systems1. But this is clearly not the case in small or shallow lakes and in estuaries, where terrestrially derived organics and photosynthesis by macrophytes and periphyton dominate organic carbon budgets.

The term "model" is no longer used because to many people it implies ecosystem simulations based on linked sets of differential or difference equations. This is quite different from what the programs described here do, viz., interpolate and extrapolate actual field data to estimate in situ photosynthesis. The terms "light", "irradiance", and "radiation" have been replaced with the more precise term "PAR", which stands for the photon flux of Photosynthetically Available Radiation. All references to the term "transparency", which was previously used to describe the attenuation of PAR a function of depth, have been replaced by the term "PAR extinction".

The algorithms used in the old programs required few modifications to bring them up to date. Here is a summary of all changes:

 As before, if data are missing from a SOL data file (PAR measured in the air), simulated cloud-free PAR values are automatically generated for the missing dates. However, previous versions used 100% of the cloud-free PAR values; the new programs use 70% of the cloud-free values, which is the percent of PAR that occurs on an average day at the Experimental Lakes Area. This percentage can be changed to a value more appropriate for other locations with the "M" run-time command (see Section 4.12).

- Cloud-free solar PAR values generated by versions of the old programs prior to 3.45 (December 21, 1987) contained a systematic error: The variation of the distance of the sun from the earth during the year was divided into the solar constant, but it should have been multiplied by the solar constant. Estimates of annual photosynthesis and mean PAR in the water column calculated from input of empirical solar data were unaffected by this error, but estimates derived from simulated "cloudless" weather could contain errors of up to 15% (J. Shearer, unpublished ELA data) and should be recalculated.
- If hypsographic (lake area as a function of depth) data are supplied, mean PAR in the water column is now calculated taking into account the diminution of the volume of the waterbody with depth. Versions of the old programs prior to 3.42 (February 11, 1987) did not incorporate this factor.
- Mean PAR in the water column is now calculated for the full 24hr day. The old programs calculated means for the period when the sun was above the horizon. The old method of calculating means can be still be selected with the "P" run-time command (see Section 4.12).
- The program used to estimate photosynthesis sis parameters from incubator photosynthesis vs PAR data is now interactive and graphical; this makes it easier to identify bad data points and results in more accurate parameter estimates.
- Users of the old programs will be relieved to know that the formats of input and output files are virtually unchanged and most data files prepared for previous versions can be rerun "as is". The only potential problem is that previously information on the line after a data type identifier in a DAT file (e.g., /ext) was ignored; this space could thus be used for recording notes (comments) about the data. The new programs do not ignore information following the data type identifier. The new convention for embedding comments is to enclose

<sup>&</sup>lt;sup>1</sup>Flynn (1989) argues that primary production should not be used as a synonym for phytoplankton photosynthesis even in these systems.

them in quotation marks (see Section 4.3.5). This is much more flexible since comments can now be placed anywhere in the DAT file, not just on the line containing the data type identifier.

- New run-time commands have been added:
  - (E)uphotic zone: Specifies the fraction of solar PAR at the bottom of the euphotic zone.
  - (F)raction: Specifies the fraction of solar PAR that occurs at the top of the water column; it is used to specify how much solar PAR penetrates through an ice cover.
  - (M)issing: Specifies the fraction of simulated cloudless PAR to use when data are missing from a SOL data file.
  - (P)artial: Causes mean PAR in the water column to be calculated only for the part of the day when the sun is above the horizon.
  - o(X)ygen: Specifies that input data are in oxygen units; causes output to be labelled in oxygen units.

These commands are fully described in Section 4.12.

• In the old IBM-PC (MS-DOS) versions of the programs, the last record in a data file was not read unless the file size was an exact multiple of 128 bytes. This was caused by a "bug" in the MS-DOS version of the PL/I compiler used to create the programs. In the new versions, which were made with Turbo Pascal, all ASCII data files are properly read.

The new programs are smaller and about twice as fast as the old ones. Error checking and messages have been improved. The manual has been rewritten and typeset.

### 2 Introduction

This report describes computer programs used to estimate in situ phytoplankton photosynthesis and mean PAR<sup>2</sup> in the water columns of lakes and oceans. These programs have evolved over a period of 20 years (Fee 1969, 1973, 1973a, 1977, 1984). The versions described here incorporate the following features:

- Daily and annual photosynthesis rates are estimated; results are expressed both in areal (per square meter) and volumetric (per cubic meter) units.
- Cloudless solar PAR can be generated for any time of year and any location on the earth.
- Separate estimates are made of photosynthesis in the mixed layer and below the thermocline.
- Daily mean PAR in the mixed layer and below the thermocline are calculated. This is useful for determining whether PAR limits photosynthesis (Hecky and Guildford 1984).
- The total mass of carbon fixed in the waterbody is calculated. This can be corrected for the fact that the volume of the lake decreases as a function of depth; Fee (1980) discusses the importance of this correction.
- The programs are based on input of photosynthesis parameters rather than tables of raw photosynthesis vs PAR data. This reduces the probability of inputting bad data and makes it suitable for estimating photosynthesis from remotely sensed chlorophyll data.

#### 2.1 Scope of the programs

Six programs are described here:

FITSOLAR: Calculates an empirical constant that describes the net effect of local atmospheric factors (e.g., haze, altitude) on incoming solar PAR. This constant makes the equations used to calculate

but we avoid this term because it implies that all photons between 400 and 700 nm result in an equal photosynthetic response, which is not the case.

<sup>&</sup>lt;sup>2</sup>The photon flux of Photosynthetically Available Radiation; defined as the number of photons between 400 and 700 nm arriving at a point. PAR is more frequently defined as Photosynthetically Active Radiation,

cloud-free solar PAR (see Section 4.3.1) appropriate for a specific location.

PSPARMS: Calculates (P)hoto(S)ynthesis (PAR)a(M)eter(S) from photosynthesis vs PAR data.

YPHOTO: Simulates (PHOTO) synthesis as a function of depth at a single place for a range of dates (usually an entire (Y) ear or ice-free season). This program is used when a lake is sampled multiple times during the year and an estimate of photosynthesis for the entire sampling period is required.

YTOTAL: Reads in the photosynthesis vs depth profiles calculated by YPHOTO and calculates integral and mean photosynthesis and mean PAR above and below the thermocline. Optionally, it corrects these (TOTAL)s for the decrease of lake volume with depth. This program provides estimates for a single location for a range of dates (usually an entire (Y)ear or ice-free season).

DPHOTO: Simulates (PHOTO) synthesis as a function of depth at a single place for a single (D)ay. This program is used to analyze data when a station is sampled only once and an estimate of photosynthesis for that day is required. Data from many different stations sampled on different days (i.e., from an entire research cruise) can be analyzed in a single run.

DTOTAL: Reads in the photosynthesis vs depth profile calculated by DPHOTO and from these data it calculates integral and mean photosynthesis and mean PAR above and below the thermocline. Optionally, it corrects these (TOTAL)s for the decrease of lake volume with depth. This program provides estimates for a single location for single dates.

Each program requires input of specific information. The information required by each of

the programs is summarized in Table 1; this table also summarizes the required units of measure for each variable.

At the Freshwater Institute these programs are used in the context of research programs that operate in the following way (complete details are given in Fee et al. 1989): In the field, samples of whole water are taken; the vertical attenuation (extinction) of PAR is measured; and PAR in the air above the waterbody (solar PAR) is measured. In the laboratory, subsamples are taken from the water sample for determining the concentrations of dissolved inorganic carbon and chlorophyll. NaH<sup>14</sup>CO<sub>3</sub> solution is added to the water, which is then siphoned into bottles. Two bottles are put in the dark, and the others are placed in a chamber having various PAR levels; they are incubated for 1-4 hr. During the incubation, PAR at each bottle position in the incubator is measured. At the end of the incubation period, <sup>14</sup>C uptake rates are determined and photosynthesis rates are calculated.

The computer programs described in this report are used to analyze these field and laboratory data: PSPARMS estimates photosynthesis parameters from chlorophyll and incubator data (photosynthesis vs PAR). YPHOTO (or DPHOTO) simulates in situ photosynthesis vs depth profiles from solar PAR, PAR extinction, chlorophyll, and photosynthesis parameter data. Finally, YTOTAL (or DTOTAL) corrects the calculated photosynthesis profiles for the decrease of lake volume with depth and estimates photosynthesis and mean PAR in the water column above and below the thermocline.

### 2.2 System requirements

The programs run on IBM-PC compatible microcomputers operating under MS-DOS (=PC-DOS) version 2 or higher. Hardware requirements are minimal: one disk drive, 192Kb of memory (RAM), and a graphics card (needed only for PSPARMS; all popular graphics cards are supported). A text editing program is needed for typing data into the disk files; any

program that can produce ASCII files will work.

### 2.3 Time requirements

The times quoted below are for an IBM-AT compatible microcomputer (Mind Computer, Winnipeg, Man.; 80286 Intel CPU running at 12 MHz; no math co-processor). FITSOLAR and PSPARMS need two to five seconds to process a single dataset. YPHOTO takes about one minute to calculate annual photosynthesis for a lake with a seven month ice-free season; YTOTAL takes about one minute to correct these results for the diminution of volume with depth. DPHOTO requires about ten seconds to calculate daily photosynthesis for a single station; DTOTAL takes about ten seconds to correct these results for the diminution of volume with depth.

### 2.4 Availability and transportability

The programs are distributed on the following IBM floppy disk formats:  $5\frac{1}{4}''$  (specify 360Kb or 1.2Mb) or  $3\frac{1}{2}''$  (specify 720Kb or 1.44Mb). They were created with Turbo Pascal (Borland International). Many extensions to the Pascal language are included in this compiler and adapting the programs to run on machines that do not have a compiler compatible with Turbo Pascal (version 4 or higher) may be difficult. Copies of the source code are included on the floppy disk along with ready to run versions of the programs.

### 3. Theory of the programs

This section describes the theoretical principles on which the programs are based. Table 4 summarizes the mathematical symbols used in this section.

### 3.1 Simulation of photosynthesis vs depth curves

The procedure used to estimate in situ photosynthesis is illustrated in Fig. 1. The re-

lationships that must be known are: (1) solar PAR (measured in the air above the waterbody) as a function of time  $(I_0 vs t; top)$ curve in Fig. 1), (2) photosynthesis as a function of PAR (P vs I; middle curve), and (3) percent of solar PAR as a function of depth (I vs z; bottom left curve, expressed as a percentage). For a given instantaneous value of  $I_0$ , the depth profile of PAR (bottom left curve) is calculated by multiplying  $I_0$  by the percent of surface PAR that reaches each depth (Ivs z). Photosynthesis as a function of depth (P vs z; bottom right curve) is then calculated from the P vs I curve in the manner illustrated. The instantaneous areal rate of photosynthesis is obtained by integrating the P vs z curve  $(\sum P = \int_0^{z_{eu}} P dz$ , where  $z_{eu}$  is the depth of the euphotic zone). The entire procedure is repeated at time intervals  $\Delta t$  (top curve) to obtain a set of instantaneous depth integrals. The daily rate is the integral of these instantaneous depth integrals over the entire day  $(\int_{sunrise}^{sunset} \sum P dt)$ . This procedure assumes that P vs I and I vs z are invariant during the day, which is not strictly true (Fee 1975; Bukata et al. 1989). However, the variations of P vs I curves are inconsistent, and Fee (1975, 1980) showed that even extreme variations have only minor effects on estimates of daily integral photosynthesis estimates. Bukata et al. (1989) concluded that diurnal changes of I vs z curves did not greatly affect daily areal photosynthesis estimates.

The heart of the calculation procedure just described is the P vs I curve. Fig. 2 illustrates how it is calculated from chlorophyll concentration (B) and two photosynthesis parameters  $P_m^B$  and  $\alpha^B$  (the superscript B indicates that  $P_m^B$  and  $\alpha^B$  are normalized on chlorophyll concentration).  $P_m^B$  is the maximum rate of photosynthesis divided by the chlorophyll concentration, and  $\alpha^B$  is the slope of the P vs I curve as PAR approaches zero divided by the chlorophyll concentration.  $P_m^B$  and  $\alpha^B$  are physiologically meaningful parameters (Bannister 1974; Jassby and Platt 1976); they are used here because the process of calculating them makes it easy to identify errors in experimental

P vs I data. Further, programs based on these parameters can be driven by remotely sensed chlorophyll data.

The equation used to describe the P vs I curve (Fig. 2) is:

$$P = \begin{cases} 0 & \text{if } I < I_k/20 \\ B P_m^B & \text{if } I \ge 2 I_k \\ B \alpha^B I' \left[ 1 - \frac{I'}{4I_k} \right] & \text{otherwise,} \end{cases}$$
 (1)

where P is the rate of photosynthesis, I is PAR,  $I_k = P_m^B/\alpha^B$ , and  $I' = I - I_k/20$ . This is adapted from an equation given in Jassby and Platt (1976). It was adopted because it can be evaluated in only 20% of the time required to evaluate their recommended hyperbolic tangent equation; both equations give identical integral photosynthesis estimates. As it is formulated, photosynthesis is zero at PAR=I'; this constant was determined empirically and corresponds to Jassby and Platt's constant  $R^B$ . Inhibition of photosynthesis by high PAR is not included in this formulation; Marra (1978), and Welschmeyer and Lorenzen (1981) have shown that such inhibition probably does not occur in situ and Fee (1980) showed that it is of little quantitative importance even if it does occur.

### 3.2 Constants

There are two groups of numeric constants—those that are permanently coded into the programs and those that can be changed at the time that the programs are run (see Section 4.12). The first group includes constants that can only be changed by editing the appropriate line in the disk file GENVARS.PAS and recompiling the programs (see Section 2.4); this is also how you can change the default value of a constant in the second group. The names given below are the actual variable names used in the file GENVARS.PAS.

The first group of constants includes:

**DELTAT:** The time interval (i.e.,  $\Delta t$ ) at which *in situ* photosynthesis is simulated during the day; thus, it is the time interval between successive values of surface

(solar) PAR in the SOL file. The default value is 30 minutes. Experiments showed no differences in daily photosynthesis estimates for values between five and 40 minutes (there were significant differences with greater values).

**MAXDATA:** The maximum number of data pairs that can appear in a single PAR extinction, chlorophyll,  $P_m^B$ ,  $\alpha^B$ , or hypsographic (area vs depth) depth profile (see Section 4.3.2). The default value is 50.

NIZERO: The maximum number of data points that can be input in a single solar PAR curve. The program uses 150, which is sufficient for a  $\Delta t$  of 10 minutes.

MINCHL, MAXCHL: As chlorophyll (B) data are read they are checked for plausibility. If a value less than 0.5 or greater than 350 is input, a warning message is issued.

MINPARM, MAXPARM: As  $\alpha^B$  and  $P_m^B$  data are read they are checked for plausibility. If a value less than 0.5 or greater than 10 is input, a warning message is issued. The values for MINPARM and MAXPARM are in carbon units; if the "X" run-time command is specified at the time the program is started (see Section 4.12) these values are multiplied by 32/12 to convert them to units of  $O_2$ .

MINYEAR, MAXYEAR: If a year specified in a DAT file is less than 1950 or greater than 2050, the run will halt.

The second group of constants includes:

ATMOS\_EFFECT ( $\kappa_a$ ): An empirical constant that specifies the fraction of solar PAR at the top of the atmosphere that reaches the surface of the earth at the location of the waterbody under cloudless conditions. It is used when YPHOTO or DPHOTO simulate cloudless solar PAR (see Section 3.5); if empirical solar PAR data are input to these programs, this

constant is not used. The default value (0.325) was measured at the Experimental Lakes Area in Northwestern Ontario. Use the program FITSOLAR to determine values for other locations.

NDEPTHS: The number of intervals that the euphotic zone is divided into, i.e., it is the number of depths on the simulated photosynthesis vs depth profile. The default value is 11. Section 3.9 describes factors that should be considered in selecting a different value.

EUPI: The fraction of surface PAR at the bottom of the euphotic zone. The default value is 0.005 (=0.5%). A warning message will be issued if the depth where this occurs is greater than 30 m.

**LATITUDE** ( $\theta$ ): The degrees from the equator (north positive) of the waterbody. It is used when YPHOTO or DPHOTO simulate cloudless solar PAR (see Section 3.5); if empirical solar PAR data are input to these programs, this constant is not used. The default value is 50°N.

### 3.3 Interpolation procedures

Linear interpolation is used to obtain values for all variables for dates between sampling dates. For example, if a chlorophyll value of 1.0 is input on June 1 and a value of 2.0 is input on July 1 then the value used on June 10 will be 1.333, on June 15 will be 1.5, and so on.

B,  $P_m^B$ , and  $\alpha^B$  data are input as functions of depth. Values for the specific depths where photosynthesis is to be calculated are obtained by linear interpolation in the input data. If the data do not encompass the depths for which values are needed, then they are extrapolated: The value at the shallowest depth that was input is used from the surface down to that depth and the value at the greatest depth that was input is used for all greater depths.

PAR extinction, and hypsographic (lake area vs depth) data are also input as functions of

depth. The run will fail if a value is not input for a depth of 0 m, or if only one value is input, or if values do not decrease with increasing depth. Values for the specific depths where photosynthesis is to be calculated are obtained by linear interpolation in the input data (PAR extinction data are linearized by taking logarithms). If it is necessary to extrapolate to greater depths than were input, a linear regression (straight line) is fit to the available data. For PAR extinction data, if five or more data points are input, the first three points are not used in fitting the straight line since the logarithm of PAR extinction vs depth is frequently nonlinear near the surface.

For all data, if only one profile is entered, it will be extrapolated forward and/or backward in time as needed. For example, if an  $\alpha^B$  depth profile dated June 1 is input and photosynthesis is calculated for the period May 1 through October 1, the June 1 value will be used for the entire period. Whenever input data are extrapolated forward or backward in time a warning message is recorded in the output.

### 3.4 Integration method

YPHOTO, DPHOTO, YTOTAL and DTO-TAL integrate functions over depth and time. All integrations are done with Simpson's 3point numerical integration rule. This algorithm consists of fitting parabolas to successive groups of three points on the curve to be integrated and summing the areas under the individual parabolas. The formula for Simpson's Rule is

$$\int_{x_a}^{x_b} f(x) dx = (x_b - x_a)[y_1 + 4y_2 + 2y_3 + \cdots + 2y_{n-2} + 4y_{n-1} + y_n]/3(n-1)$$
 (2)

where f(x) is the function being integrated,

 $x_a$  is where the integration starts, i.e. where x = a,

 $x_b$  is where the integration ends, i.e., where x = b,

 $y_k$  is the k-th value of the function f(x), i.e.,  $f(x_a) = y_1, \ldots, f(x_b) = y_n$ 

and n is the number of points at which the function is known in the interval  $(x_b - x_a)$ . Note that this algorithm requires n to be an odd number.

#### 3.5 Calculation of cloudless solar PAR

Generated solar data are scaled in units of  $mEin \cdot m^{-2} \cdot min^{-1}$  and are made specific for each waterbody by the constants LATITUDE  $(\theta)$ , and ATMOS\_EFFECT  $(\kappa_a)$ .  $\theta$  is the location of the waterbody in units of degrees from the equator (negative for the southern hemisphere) and  $\kappa_a$  is the fraction of the PAR at the top of the atmosphere that reaches the surface of the waterbody under typical cloudless conditions; its value depends on air pollution, altitude and other factors (see also Section 3.2).

The following is derived from Brock (1981). The declination of the earth during the year ( $\phi$ , the angle between the sun and the equator at solar noon, north positive) is calculated with the formula

$$\phi = 23.45^{\circ} \sin(360^{\circ}(284 + d)/\lambda_y),$$
 (3)

where d is the number of the day of the year, and  $\lambda_y$  is the number of days in the year. Letting  $k = -\tan(\theta)\tan(\phi)$ , the angle from due south of the sun at sunset  $(\varphi)$  is calculated with the formula

$$\varphi = \begin{cases} 0^{\circ} & \text{if } k > 1\\ 180^{\circ} & \text{if } k < -1\\ \arccos(k) & \text{otherwise.} \end{cases}$$
 (4)

Since the apparent movement of the sun is  $0.25^{\circ}$  of arc per minute (360°/ 1440 minutes), daylength in minutes ( $\lambda_d$ ) is simply

$$\lambda_d = 2\varphi/.25 = 8\varphi. \tag{5}$$

Using a value of 373.4 mEin·m<sup>-2</sup>·min<sup>-1</sup> for the solar constant ( $\Theta$ , the solar PAR at the top of the atmosphere at the mean solar distance), cloudless PAR at time t is calculated from the formula

$$I_0(t) = \kappa_a \Theta \delta_s^2 [\sin(\phi) \sin(\theta) + \cos(\phi) \cos(\theta) \cos(.25^{\circ}(t - \lambda_d/2))]$$
 (6)

where  $0 \le t \le \lambda_d$  and  $\delta_s^2$  is the square of the deviation of the earth from its mean distance from the sun; it is calculated from the empirical formula (Davies, 1981)

$$\delta_s^2 = 1.00011 + 0.034221\cos(k) + 0.00128\sin(k) - 0.000719\cos(2k) + 0.000077\sin(2k),$$
 (7)

where  $k = 360^{\circ} d/\lambda_y$ .

### 3.6 FITSOLAR

This program estimates the constant AT-MOS\_EFFECTS (see Section 3.2). It needs as input a date and the cloud-free PAR observed at noon on that date. The algorithm used is: (1) The upper and lower bounds for the search are set to 1 and 0. (2) The upper and lower bounds are averaged to obtain a test value. (3) A solar PAR curve is generated using the test value. (4) If the value of PAR at noon in the generated curve is greater than the observed cloud-free noon PAR value, then the upper bound for the search is set to the test value, otherwise the lower bound for the search is set to the test value. (5) Steps 2-4 are repeated until the difference between the upper and the lower bounds is less than 0.001.

### 3.7 PSPARMS

The Simplex algorithm (Caceci and Cacheris 1984) is used to find the best fit of equation 1 to the photosynthesis vs PAR data. The initial estimate of  $P_m^B$  is taken as the maximum value of photosynthesis in the dataset divided by the chlorophyll concentration; the initial estimate of  $\alpha^B$  is the slope of a straight line fit (statistical regression) of the photosynthesis vs PAR

data for all data pairs in which PAR is less than 200  $\mu \mathrm{Ein \cdot m^{-2} \cdot sec^{-1}}$ , divided by chlorophyll concentration.

### 3.8 YPHOTO and DPHOTO

These programs begin by calculating the depth of the euphotic zone (the depth where in situ PAR is 0.5% of surface PAR) from the input PAR extinction data. The euphotic zone is then divided into discrete layers of equal thickness (the number of layers is determined by the value of NDEPTHS, see Section 3.2). Before in situ photosynthesis can be simulated, values for the following variables must be known at the surface, the bottom of the euphotic zone and at the depths where the layers meet: (1) The fraction of solar PAR that reaches each depth, (2) the chlorophyll concentration (B), (3)  $P_m^B$ , and (4)  $\alpha^B$ . These values are linearly interpolated from the input data (see Section 3.3). The photosynthesis vs depth profile is then calculated according to the procedure described in Section 3.1 and integrated over depth (and time for YPHOTO) using Simpson's Rule (Section 3.4).

### 3.9 YTOTAL and DTOTAL

The functions of these programs are not incorporated into YPHOTO and DPHOTO because: (1) It would make those programs very complex and hard to modify. (2) Not every application needs to have these procedures applied. (3) More depth intervals are usually needed for YTOTAL and DTOTAL than for YPHOTO or DPHOTO (the "I" run-time command described in Section 4.12 describes how to do this). An example will make it clear why this is so: Suppose that DPHOTO calculated photosynthesis at 11 depths (the default) in a lake in which the euphotic zone was ten meters deep; photosynthesis was thus calculated at one-meter depth intervals. If the same number of intervals was used in DTOTAL to calculate the mixed layer integral and if the thermocline was at a depth of two meters, only three photosynthesis values would be used for calculating the mixed layer integral; this would be very inaccurate. However, if you tell DTOTAL to use 41 depth intervals, nine data points will be used for calculating the mixed layer integral, giving similar accuracy for the 0-2 m integral as was obtained for 0-10 m integral in DPHOTO.

Like YPHOTO and DPHOTO, these programs divide the euphotic zone into discrete layers of equal thickness and calculate values for the following variables at the surface, at the bottom of the euphotic zone and at each of the depths where the layers meet: (1) The fraction of solar PAR that reaches each depth, (2) the daily photosynthesis at each depth, (3) the area of the lake at each depth (if hypsographic data are input). In addition, the depth of the mixed layer must be known. Given all of the required variables, it is straightforward to calculate the various integrals with Simpson's Rule (Section 3.4).

### 4 Using the Programs

### 4.1 Disk files

Except for FITSOLAR, which reads its input from the keyboard and displays its results on the computer monitor, the programs read their inputs from disk files and write their outputs into other disk files. MS-DOS file names contain two parts separated by a period (e.g., NAME.EXT). The part before the period is the primary file name (hereafter referred to as NAME); it can contain eight or fewer characters. The part after the period is called the extension (hereafter referred to as EXT); it can contain three or fewer characters. In general, you choose the file NAME<sup>3</sup>—it identifies the location or cruise that produced the data contained in the file. For example, you could choose the NAME "GREEN89" for the file that contains data from Green Lake in 1989. The file EXT, on the other hand, identifies the kind of information contained in a file (e.g., files with an EXT of "SOL" contain solar PAR

<sup>&</sup>lt;sup>3</sup>The only exception is for solar data, where the file NAME identifies the year. See Section 4.3.1.

data, and files with an EXT of "OUT" contain simulated photosynthesis profiles). The files you create must have the correct EXTs or they will not be found by the programs. Table 2 summarizes all of the file types used in the programs, giving the EXT and a description of what file contains. Table 3 summarizes the file types read as input and produced as output by each program.

The programs all read their input data in "free-format"; this means that it does not matter where you type data on an input line—successive values can be separated by blanks, commas, tabs, or the ends of lines, and alphabetic data can be entered in either upper or lower case. However, data must appear in the file in the proper order. For example, dates are input as the month name followed by the day of the month (e.g., Aug 1; only the first three letters of the month name are necessary). If you enter this date with the month and day reversed (i.e., 1 Aug) the programs will fail.

The first non-blank line in any disk file is simply copied to the top of the output files; it serves to identify the output. You can put any information that you want on this "header" line, but be sure that the location and time period are included so that the output will be understandable.

### 4.2 Error Handling

If YPHOTO, YTOTAL, DPHOTO, or DTOTAL fail for a known reason, a message describing the problem will be displayed on the screen. This message will also be permanently stored in a disk file with the same NAME as the NAME of the input DAT file and an EXT of "###". This facilitates the use of the programs in DOS batch files: If you submit several runs to DOS for execution in a single batch file you can find out which (if any) of the runs failed simply by typing the DOS command "DIR \*.###".

If an unforeseen error occurs, the program will stop, displaying the message "Runtime error nnn at xxxx:yyyy". This is an emergency message produced by Turbo Pascal; nnn

is the runtime error number, and xxxx:yyyy is the address of the error. Detailed explanations of runtime error messages are given in the Turbo Pascal manual. However, the cause of a problem will usually be obvious: e.g., the disk is full. If you cannot figure out why the program failed, please send a disk containing a copy of the dataset that caused the error along with a copy of the error message to the author.

If a run terminates abnormally, e.g., if the electrical power fails or if you get a runtime error message from Turbo Pascal, files with an EXT of "%%%" will appear in your disk directory. These are temporary files that will be erased automatically if you restart the interrupted run; you may safely erase them by typing "DEL \*.%%%".

Input data are carefully scrutinized for plausibility. If a questionable value (using the criteria described in Section 3.2) is found, the run continues but a warning message is recorded in any output computed from this datum.

### 4.3 Data Used by More than one Program

### 4.3.1 Solar data

YPHOTO, YTOTAL, DPHOTO or DTOTAL first try to read solar data from a disk file whose NAME is the year for which calculations are to be made and whose EXT is "SOL" (e.g., 1976.SOL). If this file cannot be found, the programs next search for a file called CLDLSS.SOL. If neither of these files is found, then the algorithms described in Section 3.5 are used to simulate solar PAR. Calculating solar PAR for an entire ice-free season or year can take considerable time. For efficiency, solar data generated by YPHOTO are stored in a file named CLDLSS.SOL; subsequent runs will read solar PAR data from this file.

Solar data are input as tables (one for each day) that give the instantaneous flux of solar PAR at time intervals of 30 minutes. Data are required only for times when the sun is above the horizon, but including zeros for the dark periods does no harm. A solar file containing

data for two days follows:

```
ELA cloudless solar PAR data.
May 1
  0.0
      11.9 18.8 27.0 36.2 46.0
                                  56.2
      76.4 85.9
                  94.4 101.7 107.7 112.2
114.9 115.8 114.9 112.2 107.7 101.7
           66.5
                 56.2
                        46.0
                             36.2
      76.4
 18.8
       11.9
             0.0
May 2
  0.0
      11.8 18.4
                  26.3
                        35.1 44.6
 64.4 74.2 83.6 92.1
                        99.7 106.1 111.0
114.4 116.1 116.1 114.4 111.0 106.1
                        54.5 44.6
 92.1 83.6 74.2 64.4
 26.3
      18.4 11.8
                   0.0
                        -1
```

The file starts with a header line. The data for each day begins with the date. Following the date come the data for that day. A negative value where a PAR value is expected is the signal that all data for that day have been entered. The data in a SOL file must appear in chronological order but it is not necessary that the file contain data for every consecutive day; i.e., the file can contain gaps. Missing data are generated using the algorithm described in Section 3.5; a warning message is recorded in the output whenever this is done. Theoretical cloud-free PAR values are multiplied by 0.7 to simulate average cloudiness. This is the fraction of full solar PAR that occurs on an average day at the Experimental Lakes Area (NW Ontario); more appropriate values for other locations can be specified with the "M" run-time command (see Section 4.12).

### 4.3.2 PAR extinction, $P_m^B$ , $\alpha^B$ , and chlorophyll data

These data are input as depth profiles. Each depth profile starts with the date. Following the date are pairs of data; the first number in each pair is taken to be a depth, the second number is taken to be the value of the variable at that depth. A negative value where a depth is expected is the signal that all data for the profile have been entered. For example, a single depth profile of PAR extinction follows:

2 25 3 12.5

4 6.25

-:

Because data entry is free-format, these data could also be input as:

July 17 0 100,1 50,2 25,3 12.5,4 6.25 -1

Notice that no header lines are shown in these examples. This is because depth profile data are always input as part of a DAT file; only the first line of the DAT file contains a header line. Note further that the PRM output file generated by PSPARMS is not in the proper format for input of B,  $P_m^B$ , or  $\alpha^B$  data.

### 4.3.3 Hypsographic (lake area vs depth) data

If you want YTOTAL or DTOTAL to correct the photosynthesis values for the decrease of the volume of the lake with depth, then you must supply hypsographic data. The format of these data is the same as for depth profile data (Section 4.3.2) except that no date is attached to them. A sample dataset looks like:

0 27.7E8 2 24.47E8 4 23.90E8 6 21.29E8 8 17.37E8 10 10.74E8 12 0.65E8 -1

The first number in each pair is the depth, the second is the area of the lake at that depth in units of meters<sup>2</sup>.

#### 4.3.4 Mixing depth data

YTOTAL and DTOTAL need input of the mixing depth in order to calculate photosynthesis above and below the thermocline. An example mixing depth dataset follows:

Apr 1 5 May 1 3

May 5 6

May 30 10

Note that there is no negative "end of data" signal separating data for different dates as appeared in the chlorophyll,  $P_m^B$ , and  $\alpha^B$  dataset in Section 4.3.2; it is not needed because only one value of mixing depth is input for each date. If mixing depths are specified that are

July 17

<sup>0 100</sup> 

<sup>1 50</sup> 

greater than the depths to which photosynthesis was computed then YTOTAL (or DTOTAL) will extrapolate the latter as necessary to obtain values for greater depths. If mixing depths greater than the maximum depth in the hypsographic data are specified, then the latter will be used for for the mixing depth.

### 4.3.5 Organization of data in DAT files

YPHOTO, YTOTAL, DPHOTO and DTOTAL read several types of data from a data file whose EXT is "DAT". These different data types (PAR extinction, chlorophyll,  $\alpha^B$ ,  $P_m^B$ , mixing depth, hypsographic data) can be entered in any order in a DAT file. Each data type is separated from the others by a line which has a slash (/) followed by three letters, which specify the type of data which follow (ext = PAR extinction, chl = chlorophyll, alp =  $\alpha^B$ , pbm =  $P_m^B$ , zep = mixing depth, hyp = hypsographic data). See Sections 4.7—4.8 for examples.

In the previous version of these programs, any information on the line after the data type identifier (e.g., /ext) was ignored; this space could thus be used for recording notes (comments) about the data. In the new version, information on this line is *not* ignored. The new way of commenting data is to enclose them in quotes (either single or double quotation marks can be used, but the quotation marks must be properly paired; a comment may not extend beyond the end of a line). Comments can appear anywhere inside PAR extinction, chlorophyll,  $\alpha^B$ ,  $P_m^B$ , mixing depth, or hypsographic data; Section 4.8 gives examples.

### 4.4 Starting the Programs

All of the programs are started by typing the name of the program, a space and then the NAME of the disk file (see Section 4.1) that contains input data for that program. For example, to start the program YPHOTO and tell it that the input data are to be found in the disk file ELA84.DAT you would type:

A>YPHOTO ela84

The symbols "A>" are the DOS system prompt, you type the rest (in this and all examples which follow, text that you type is underlined). Each program starts by printing its name, the version number, and the date on which it was created. While a program is running it may print informative messages on the screen. For example, YPHOTO may print:

Generating cloudless PAR data... Press B to breakpoint run

The first line indicates that a disk file with solar data could not be found so these data were generated; the last line indicates that you may interrupt the program by pressing "B" on the keyboard.

#### 4.5 FITSOLAR

This program prompts the user to type in the date, latitude, and the measured value of PAR at midday under cloudless weather. It displays the fitted value of ATMOS\_EFFECTS on the console monitor. Shown below is a complete session with this program.

#### A>fitsolar

FITSOLAR Version 4.0 <date created>
FWI Software Tools

Enter year (e.g. 1980): 1984 Enter latitude in degrees: 50

Enter month (e.g. May): jun
Enter day (e.g. 1): 1
Enter surface PAR at noon: 125.5
ATMOS\_EFFECT = 0.3917

Enter date (e.g. May 1): ^C

The symbol "C" stands for Control-C and is obtained by pressing the Break key while holding down the "control" key. This is the way that you terminate the program.

#### 4.6 PSPARMS

This program reads chlorophyll concentration and photosynthesis vs PAR data from a disk file whose EXT is INC. For each dataset the input data and the fitted mathematical curve (Fig. 2) are displayed on the screen. The user is then given the option to exclude individual data points with the aim of achieving the best fit of the curve to the experimental data. Final parameter values are stored in a disk file having the same NAME as the input file and an EXT of PRM. An example data file containing two datasets follows:

Yellowk	nife Lal	ke Stud	y, 1983	Data
Station	-01 5.7			•
13	-1	0.14	-9	
39.2	-1	0.67	0.78	-9
126.7	-1	2.49	3.05	-9
366.7	<b>-1</b>	3.05	3.13	-9
-1				
'Statio	n 75 5	-Ju1-83	2.6	
10.1	12.4	-1	0.11	-9
27.3	-1	0.57	0.57	-9
57.5	-1	1.49	1.62	-9
125.6	-1	5.36	3.57	-9
289.2	-1	4.80	-9	
-1				

These data are interpreted in the following way: The first line in the file is a header that is copied to the top of the output PRM file. Each incubator dataset starts with an identifier (e.g., Station-01), which can contain 30 or less characters (if it is longer than this it will be truncated). If the identifier contains blanks, it must be enclosed in quotes, as shown in the second dataset. The number following the dataset identifier is taken to be the chlorophyll concentration. PAR measured in the incubator at the position of the first bottle follows the chlorophyll concentration; the end of the replicate PAR measurements is signalled by a negative number. The replicate PAR measurements are averaged to obtain a single value that will be associated with the photosynthesis rates measured at this PAR. After PAR come photosynthesis rates measured at this PAR value. Successive numbers are read until one less than or equal to -5 is encountered; negative photosynthesis values greater than this can be input but are not used in the curve fitting procedure. The replicate photosynthesis rates measured at a single value of PAR are not averaged. The above format (PAR values followed by photosynthesis values) is repeated for each position in the incubator. A negative number where a PAR value is expected terminates data input for the dataset. Up to 128 photosynthesis rates can be input in a single dataset. PvsI data can be entered in any order, i.e., from low PAR to high or vice versa.

If the data shown above are in a file called TESTPRM.INC, then typing

### A>psparms testprm

starts the program. The input data from the first dataset are graphed on the screen, along with the fitted PvsI curve. When you press the ENTER key, the data are displayed in tabular form along with a menu of options:

(D)rop point, (G)raph, (A)bort, (C)ontinue

Choose an option by pressing the letter enclosed in parentheses:

- (D)rop point The program will ask you which point to drop. Enter the sequence number of the point. If you select a point twice it will be "undropped", i.e., re-included in the dataset for fitting the curve.
- (G)raph The data will be redisplayed, with dropped data points circled.
- (A)bort The run will be terminated immediately. You may want to do this if you need to make corrections to data.
- (C)ontinue If you have dropped any data points, the Pvs I curve will be refit and the data with the new curve will be redisplayed. If you did not drop any data points, then the program will proceed to the next dataset.

It is an unfortunate fact that human judgement is a necessary part of the process of estimating  $P_m^B$  and  $\alpha^B$ . The previous version of this program fully automated this process, but it became apparent that a single bad data point in an otherwise good dataset could result in very inaccurate parameter estimates. Fortunately, it is easy to identify bad data points when the photosynthesis vs PAR data are shown graphically. Obviously, data should

be dropped with caution, and you should make permanent copies of the final graphs so that you will have a permanent record of what data were used. You can do this by pressing the Shift-PrintScreen key combination at any time that a graph is displayed on the screen. DOS supplies a program (GRAPHICS.COM) for this purpose (see your DOS manual for a description of how to use this program), but it does not work with all graphics cards or printers. The program Pizzaz (Application Techniques, Inc.) is a better print-screen program that works with all popular cards and printers; it also offers much more flexibility than GRAPHICS.COM (smoothing, placement on the page, scaling the graph to a specific size, printing to a file, etc.).

If the above example is run and no data points are dropped, PSARMS will produce a disk file called TESTPRM.PRM which is shown in Fig. 3. This file contains the following information: The first three lines are the run identifier (header) and column labels; following this come the results, one line per dataset. Column 1 is the dataset identifier. Column 2 is the number of iterations required for convergence to a solution; small numbers mean that a solution was found quickly. If the number is 100 it means that convergence was not obtained. Column 3 is the chlorophyll concentration. Column 4 is the estimate of  $P_m^B$ . Column 5 is the estimate of  $\alpha^B$ . Column 6 is the sum of the squares of the deviations of the photosynthesis equation to the experimental data; the higher this number, the worse the fit.

#### 4.7 YPHOTO

This program reads data from two disk files: (1) A SOL file containing PAR values in air for the period for which photosynthesis is to be calculated (see Section 4.3.1). (2) A DAT file (see Section 4.3.5) containing a header line, the starting and ending dates for which calculations are to be made, and depth profiles of chlorophyll, PAR extinction,  $\alpha^B$  and  $P_m^B$ . An example DAT file for YPHOTO looks like:

```
May 1, May 10, 1976
/ext
May 5
         0 100
                  10
                                -1
/chl
May 1
                  -1
             1
May 10
            10
                  -1
/alp
Jan 1
         0
             5
                  -1
/pbm
Dec 31
         0 1.98
                  -1
```

This file is interpreted in the following way: The first line is a header. The starting and ending dates for which photosynthesis is to be calculated follow; these dates must both be in the same year and separate runs must be made if the period for which photosynthesis is to be calculated extends past the end of a year (e.g., photosynthesis for the period Oct 20, 1976 to Mar 31, 1977 would have to be done in two runs: Oct 20, Dec 31, 1976 and Jan 1, Mar 31, 1977). The year for which photosynthesis is to be calculated is input next. Depth profiles of PAR extinction, chlorophyll,  $\alpha^B$  and  $P_m^B$  follow. See Section 4.3.5 for a description of the organization of these data in DAT files.

If the data shown above are in a file called TESTYR.DAT and if neither 1976.SOL nor CLDLSS.SOL can be found on the disk, then typing

### A>YPHOTO testyr

will produce a disk file called CLDLSS.SOL that contains simulated cloudless PAR values for the period for which photosynthesis was simulated (Fig. 4). A second file (called TESTYR.OUT) will also be produced. This file will contain the following information: For each day, the depth profile of photosynthesis and the integral of this curve over depth. The depth profile of photosynthesis for the entire time period for which calculations were made and the integral of this curve over depth follow. Finally, the values of the input data that were used at each depth where photosynthesis was calculated and warning messages (if any) are summarized. Fig. 5 shows the output produced from the example dataset.

### 4.8 YTOTAL

This program requires the same input data files that YPHOTO required. In addition it reads the OUT file produced by YPHOTO. The DAT file must contain mixing depth (see Section 4.3.4) data. If you wish to have the totals corrected for the diminution of lake volume with depth, the DAT file must also contain hypsographic data (see Section 4.3.3). An example DAT file for YTOTAL looks like:

```
Lake Winnipeg 1976, Cruise 3
May 1, May 10, 1976
/ext
May 5
        0 100
/chl 'this is a comment'
                   "another comment"
        0
            1 -1
May 10
        0
           10 -1
/alp
            5
Jan 1
/pbm
Dec 31 0 1.98 -1
/hyp
0 27.78E8, 2 25.57E8, 4 23.90E8, 6 21.29E8,
8 17.37E8, 10 10.74E8, 12 0.65E8 -1
/zep
      1 3
May
    30 10
May
```

The structure of this DAT file is the same as that described for YPHOTO (Section 4.3.5 gives a more detailed description of the organization of data in DAT files). Note that this DAT file contains more data than the one given as an example in Section 4.7. Actually, the same DAT file can be used as input to both YPHOTO and YTOTAL, with all data needed by both programs included; each program will simply ignore data in the file that it does not use.

If the files TESTYR.OUT and CLDLSS.SOL produced by the example shown in Section 4.7 are on the disk, and if the data shown above are contained in the file TESTYR.DAT, then typing

### A>YTOTAL testyr, i=41

will produce a file called TESTYR.TOT shown in Fig. 6. This file contains the following results: For each day, the mixed layer depth; uncorrected and (if hypsographic data were input) corrected integrals of photosynthesis over depth; average photosynthesis (per meter<sup>3</sup>) above and below the thermocline, and mean PAR above and below the thermocline. This is followed by integrals and averages for the entire time period for which calculations were made. Finally, warning messages (if any) are summarized.

Note in the example output that the uncorrected integrals (col. 4) do not exactly match the corresponding results in the file TESTYR.OUT (Section 4.7); this is because the integrals reported by YTOTAL were calculated with 41 depth intervals while those calculated by YPHOTO were calculated with only 11 depth intervals. The reason for using more depth intervals in YTOTAL and DTOTAL than in YPHOTO and DPHOTO was discussed in Section 3.9.

### 4.9 DPHOTO

In addition to the input files required by YPHOTO (described in Section 4.7), this program needs a STA file, which contains a header line for the entire run, followed by a list of NAMEs of disk files (one per station). An example STA file follows:

```
Lake Winnipeg 1976, Cruise 3
```

The first line is a header. The character strings on the following lines (any number can be input; for simplicity, only one is shown here) are the NAMEs of DAT files, that contain the input data for the named station. In this example DPHOTO would search for a file named 318.DAT; which contains the following data:

```
L. Wpg, Sta 318, 1976 Cloudless weather
Jun 6, 1976
/ext 'this is a comment'
Jun 6 0 100 2 2.19 -1
/chl
Jun 6 0 1.7 -1 "another comment"
/alp
Jun 6 0 5.4 -1
/pbm
Jun 6 0 4.7 -1
```

The format of this DAT file is identical to the DAT files input to YPHOTO (see Section 4.7) except that only one date is specified on the second line instead of a range of dates. If a date of any data in the DAT file does not match the date for which photosynthesis is to be calculated, then a warning message is recorded along with the computed results. The output is the same as for YPHOTO (see Section 4.7) except that only results for a single date appear.

If the data sets shown above are in the disk files TESTDAY.DAT and 318.STA, and if there are no solar data on the disk then typing

### A>DPHOTO testday

will produce the output shown in Fig. 7 in the file TESTDAY.OUT.

#### 4.10 DTOTAL

This program requires the same input data files required for input to DPHOTO; in addition, it reads the output file produced by DPHOTO. The DAT file must contain mixing depth (see Section 4.3.4 for the format of these data) and hypsographic data (see Section 4.3.3 for the format of these data); the hypsographic data can be omitted if you do not wish to have the totals corrected for the diminution of volume with depth.

The STA file for use with DTOTAL would look exactly like the example given in section 4.9. The file 318.DAT pointed to by this example contains the following information:

L. Wpg,	Sta 3	18, 1976	Cloud	Less weath	ıer
Jun 6,	1976				
/ext					
Jun 6	0	100	2	2.19	-1
/chl					
Jun 6	0	1.7	-1		
/alp					
Jun 6	0	5.4	-1		
/pbm					
Jun 6	0	4.7	-1		
/hyp					
0 27.78	BE8, 2	25.57E8,	4 23.9	90E8, 6 21	.29E8,
8 17.37	7E8, 10	10.74E8	, 12 0	.65E8 -1	
/zep					
Jun 6	10.0				

As with the YTOTAL example data set (see Section 4.8), this DAT file contains more data than the DAT file given as an example in Section 4.9. Normally the same DAT file is used as input to both DPHOTO and DTOTAL, with all data needed by both programs included; data that are not needed are simply ignored.

If the disk contains the TESTDAY.OUT file produced by the example in Section 4.9 and if the example data shown in above are contained in the file TESTDAY.DAT then typing

### A>DTOTAL testday, i=41

will produce a file called TESTDAY.TOT, shown in Fig. 8.

### 4.11 Breakpointing Runs

YPHOTO and DPHOTO can be interrupted and subsequently restarted without losing intermediate results. This allows you to ensure that there are no errors in the data before calculating photosynthesis for an entire year; it is also convenient to be able to interrupt a long run if you need the computer for something You breakpoint a run by pressing the letter "B" anytime after the message "Press B to breakpoint run" appears on the screen (see Section 4.4) or by using the "B" run-time command (see Section 4.12). When you breakpoint a run, intermediate results are stored in three disk files: (1) NAME.OUT contains the photosynthesis profiles calculated up to the breakpoint, (2) NAME.### contains diagnostic messages, and (3) NAME.BRK contains intermediate results needed to restart the run. If any of these files cannot be found when you restart the run, the others will be erased and calculations will start over from the beginning.

### 4.12 Run-time commands

The programs incorporate specific values for variables that vary from place to place; they also perform some calculations in ways that may not be universally applicable. By appending certain letters to the NAME of the data file when you start a program, you can alter these constants and calculation procedures to make

them apply to your situation. These run-time commands are separated from the file NAME and from each other by spaces and/or commas (see examples below). In the following command descriptions, names enclosed in angle brackets (<>) are to be replaced with actual values (e.g., you might type "101" where <ndepths> appears); items enclosed in square brackets ("[]") are optional. The letter enclosed in parentheses is what you type on the command line to select the option. Currently implemented run-time commands are:

- (A)tmos\_Effect=<value>: The number after the equal sign will be used as the value of ATMOS\_EFFECT (see Section 3.2).
- (B)reakpoint: Causes YPHOTO to breakpoint (see Section 4.11) after checking the input data for errors and computing photosynthesis for the first day. This allows you to check for bad input data, to see the depths at which calculations are going to be made, and to check the magnitude of the calculated results on the first day before committing the computer to a long calculation.
- (C)heck: Forces YPHOTO to check the solar data for errors before starting the calculations. YPHOTO does not normally check the solar data for errors (as it does all of the other input data) because a single solar PAR dataset is typically used for many different stations or for many different lakes. It takes about five times as long to read and check these data during the preliminary error checking phase of the program than it does to check all the other input data combined. Moreover, it is only necessary to check these data once (or indeed to not check them at all, e.g., when the program is using simulated cloudless weather).
- (E)uphotic zone=<number>: Specifies the fraction of surface PAR at the bottom of the euphotic zone. The default value is 0.005(=0.5%). <number> must be input as a fraction, i.e., a number less than 1.

- (F)raction=<number>: Specifies the fraction of solar PAR (measured in air) remaining at the top of the water column. The default value is 1.0; this value will need to be changed only if the waterbody is covered by ice and snow, which absorb PAR. <number> must be input as a fraction, i.e., a number less than 1.
- (I)ntervals=<ndepths>: The number after the equal sign will be used as the value of NDEPTHS (see Sections 3.2 and 3.9). The default value is 11. Because of the integration algorithm used (see Section 3.4), <ndepths> must be an odd number. To assure reasonable accuracy, values less than five are not allowed. If more than 101 intervals are needed, then the program must be recompiled after changing the value of MAXINTR in the file GEN-VARS.PAS (see Section 2.4).
- (L)atitude=<degrees>: The number after the equal sign will be used as the value of LATITUDE (see Section 3.2). This value is used when solar PAR values are simulated; it is irrelevant if you are using empirical solar PAR data which contain no missing data. Enter values for the southern hemisphere as negative numbers.
- (M)issing=<number>: If data are missing from a SOL data file, solar PAR values will be simulated by the programs. This option is used to specify the fraction of the theoretical cloud-free PAR that reaches the surface of the lake on an day with average cloudiness. The default value is 0.7 (=70%); it was measured at the Experimental Lakes Area in Northwestern Ontario and will not be appropriate for waterbodies located in sunnier or cloudier climates. <number> must be input as a fraction, i.e., a number less than 1.
- (O)utput=<drive>: This command specifies the letter of the disk drive (see the DOS manual for the disk drive nomenclature) where you want the output file(s)

stored. If you do not specify otherwise, the output files will be written onto the drive that contains the input files.

- (P)artial: This causes YTOTAL and DTO-TAL to calculate mean PAR in the water column only for the part of the day during which the sun is above the horizon. This was the way that previous versions of these programs worked (the default now is to calculate averages for the entire 24 hr day).
- (S)olar=<drive>: This command allows you to specify which disk drive contains the solar PAR data. By putting the solar data on a different drive, you can make more space available on the default drive for output files.
- (U)niform: This causes the input data values for B (chlorophyll),  $\alpha^B$  and  $P_m^B$  to be applied uniformly over the input depths instead of being linearly interpolated. An example will make this clear: Suppose that the input data looked like:

### MAY 5 0.0 10, 5.0 100, 10.0 1000, -1

If the (U)niform command is given, then all depths between 0 and 5 meters will be assigned the value 10, all depths between 5 and 10 meters will be assigned the value 100 and any depths greater than 10 meters will be assigned the value 1000. If you do not specify this command then values will be linearly interpolated: if calculation depths are at 0, 1, 2, etc. then the interpolated values for the above dataset would be 10, 28, 46, etc. For this reason, "U" should be specified whenever integrated samples are taken.

- o(X)ygen: Specifies that photosynthesis input data  $(P_m^B \text{ and } \alpha^B)$  are in oxygen units; causes output to be labelled properly.
- (Z)max[=<maxdepth>]: This command forces the program to use the maximum depth appearing in the PAR extinction

data as the depth of the euphotic zone. It is needed in shallow lakes, where the euphotic zone depth calculated from the PAR extinction data is greater than the actual maximum depth of the lake. Optionally, you can specify the euphotic zone depth by including an equal sign followed by a number (assumed to be a depth, in meters).

Some examples are:

### A>YPHOTO ELA84,Z,B,I=15

This run will use the maximum depth in the input PAR extinction data as the depth of the lake, it will calculate photosynthesis at 15 depth intervals and it will automatically breakpoint itself after calculating photosynthesis for the first day.

### A>YPHOTO WPG76,Z=10.5,L=53,C,S=B,O=C,P

This run will use 10.5 meters as the maximum depth, 53 degrees for the latitude if cloudless PAR values are calculated, the solar PAR data will be checked for errors before doing the calculations, solar PAR data will be read from disk drive B, the output file (WPG76.OUT) will be written on drive C. The "P" option (which is used to tell YTOTAL to calculate mean PAR in the water column only for the part of the day when the sun is above the horizon) is ignored by YPHOTO.

### 4.13 Unusual problems

This section describes some unusual situations that may arise and presents solutions.

• If a run of YPHOTO in a batch file fails, the error messages are stored in a file with an extension of '###'. If the batch file then runs YTOTAL on the same dataset, the '###' file created by YTOTAL will overwrite the '###' file created by YPHOTO (the same applies to sequential runs of DPHOTO and DTOTAL). This happens because both programs use the same EXT (###) for storing fatal error messages. You can prevent this by putting "IF NOT EXIST <filename>.###" at the beginning of

the line in the batch file that runs YTO-TAL, where <filename> is the NAME of the DAT (or STA) file; this will cause DOS to ignore the command if the previous run failed.

- Chlorophyll data might be unavailable for a station where the photosynthesis vs PAR data were measured. Without chlorophyll data,  $P_m^B$  and  $\alpha^B$  cannot be estimated, and without these parameters, in situ rates cannot be calculated. This means that the photosynthesis vs PAR data will be wasted. However, the chlorophyll values that are used to estimate  $P_m^B$  and  $\alpha^B$ are later "factored out" when in situ rates are calculated (study Section 3.1 and you will see why this is so). Therefore, so long as the chlorophyll,  $P_m^B$  or  $\alpha^B$  values are not used for any purpose other than estimating in situ photosynthesis, a dummy value of chlorophyll (1.0) can be used for estimating  $P_m^B$  and  $\alpha^B$ .
- It would be helpful in some lakes if the "U" option (see Section 4.12) could be invoked in the mixed layer and then "turned off" for samples in the metalimnion and hypolimnion. This can be achieved by inputting the mixed layer data twice, assigning a depth of zero to the first dataset and the depth of the mixed layer to the second dataset.

### 5 Acknowledgments

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Table 1. The data used in the programs, required units, and which programs use them.

Data	Units	Used by
Latitude	degrees (north positive)	FITSOLAR
Midday PAR	$mEin^{\dagger} \cdot m^{-2} \cdot min^{-1}$	FITSOLAR
Incubator PAR	$\mu \mathrm{Ein} \cdot \mathrm{m}^{-2} \cdot \mathrm{sec}^{-1}$	PSPARMS
Photosynthesis Rate	$mg C \cdot m^{-3} \cdot hr^{-1}$	PSPARMS
Solar PAR	mEin·m <sup>-2</sup> ·min <sup>-1</sup>	<b>ҮРНОТО</b> , <b>РНОТО</b> ,
		YTOTAL, DTOTAL
In situ PAR extinction	any units	<b>ҮРНОТО</b> , <b>РНОТО</b> ,
		YTOTAL, DTOTAL
Chlorophyll $(B)$	$ m mgchl\cdot m^{-3}$	PSPARMS,
		<b>ҮРНОТО</b> , <b>ДРНОТО</b> ,
_		YTOTAL, DTOTAL
$lpha^B$	$\operatorname{mg} C (\operatorname{or} O_2) \cdot \operatorname{mg} \operatorname{chl}^{-1} \cdot \operatorname{Ein}^{-1} \cdot \operatorname{m}^2$	<b>ҮРНОТО</b> , <b>DРНОТО</b>
$P_m^B$	$\operatorname{mg} \operatorname{C} (\operatorname{or} \operatorname{O}_2) \cdot \operatorname{mg} \operatorname{chl}^{-1} \cdot \operatorname{hr}^{-1}$	<b>ҮРНОТО</b> , <b>РРНОТО</b>
Mixing depth	m	${f YTOTAL},{f DTOTAL}$
Hypsographic (area vs depth) data	$m^2$	YTOTAL, DTOTAL
<sup>†</sup> An Einstein is 1 mole of photons.	•	

Table 2. The file EXTensions used in the programs and the kind of data contained in each.

File EXTension	Contents
INC	Chlorophyll and photosynthesis vs PAR data
PRM	Estimates of $P_m^B$ and $\alpha^B$
SOL	Solar PAR (measured in air)
DAT	Depth profiles of PAR extinction, $P_m^B$ , $\alpha^B$ , chlorophyll, and area; mixing depth
STA	List of the NAMEs of DAT disk files; one for each station
OUT	Simulated in situ photosynthesis depth profiles and integrals of these profiles over depth
TOT	Integrals of photosynthesis and mean PAR for the water columns above and below the thermocline (optionally corrected for the decrease of lake volume with depth)
*##	Error messages. Files with this EXTension are produced only if an unrecoverable error occurs or if a run is breakpointed
BRK	Breakpoint information. Files with this EXTension are produced if a run is interrupted

Table 3. Summary of file EXTensions read as input and produced as output by each program. EXTension names enclosed in square brackets are files produced only under special circumstances: [SOL] is produced if one is not found; [###] is produced if a run fails or is interrupted; [BRK] is produced if a run is interrupted. Table 2 explains what kind of information each file EXT contains.

Program	Input File EXT	Output File EXT
PSPARMS	INC	PRM
<b>ҮРНОТО</b>	SOL, DAT	OUT, [SOL], [###], [BRK]
YTOTAL	SOL, $DAT$ , $OUT$	TOT, [###]
DPHOTO	SOL, DAT, STA	OUT, [###], [BRK]
DTOTAL	SOL, DAT, STA, OUT	TOT, [###]

Table 4. Definitions of mathemathical symbols.

$\overline{B}$	chlorophyll concentration
$P_m^B \ lpha^B$	the rate of photosynthesis at optimal PAR divided by $B$
$lpha^{\overline{B}}$	the slope of the photosynthesis vs PAR curve at low PAR values, divided by B
<b>P</b>	the rate of photosynthesis
I	PAR, the photon flux of photosynthetically available radiation
t	time
f(x)	function $f$ of variable $x$
Ivsz	I as a function of depth, i.e., $I(z)$
$I_0  vs  t$	$I$ as a function of time, i.e., $I_0(t)$
$P \ vs \ z$	photosynthesis as a function of depth, i.e., $P(z)$
P  vs  I	photosynthesis as a function of $I$ , i.e., $P(I)$
$z_{eu}$	the depth of the euphotic zone (where photosynthesis = respiration)
$I_0$	I measured in the air above the waterbody
$I_k$	$P_m^B/~lpha^B$
I'	$I-I_k/20$
$\Delta t$	time between $I_0$ data; the basic time step in the simulation of daily photosynthesis
$\kappa_a$	the fraction of $I$ at the top of the atmosphere that reaches the surface of the
	waterbody under cloud-free conditions
$\theta$	distance of the waterbody from the equator (degrees, north positive)
$\boldsymbol{z}$	$depth, z_a is depth = a, z_b is depth = b$
$y_k$	the $k$ -th value of function $y$
$\boldsymbol{n}$	the number data points
$oldsymbol{\phi}$	the angle between the sun and the equator at solar noon
d	the number of the day of the year
$\lambda_y$	the number of days in the year
$\boldsymbol{k}$	a constant, variously defined in the text
arphi	the angle of the sun from due south at sunset
$\lambda_d$	${\bf daylength}$
Θ	I at the top of the atmosphere at the mean solar distance
$\delta_s^2$	the square of the deviation of the earth from its mean distance from the sun

Fig. 1. The procedure used to estimate in situ photosynthesis. See Section 3.1 for a detailed explanation.

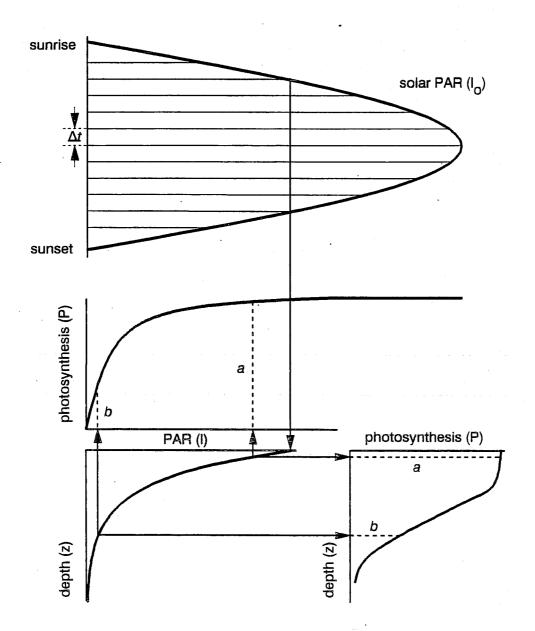


Fig. 2. The photosynthesis vs PAR curve, illustrating the equation used and graphically defining the photosynthesis parameters.

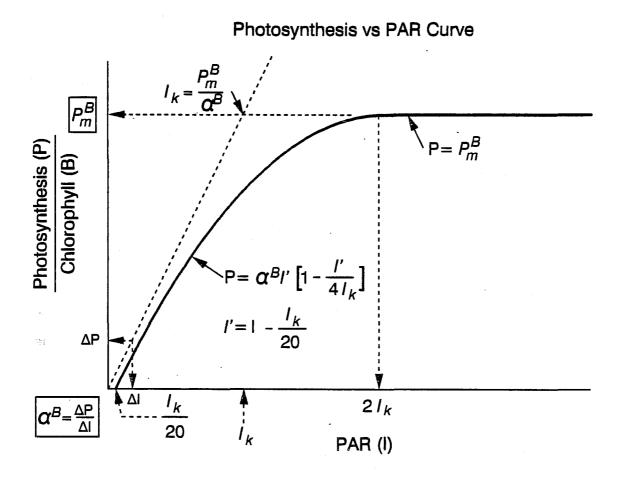


Fig. 3. Example output from the program PSPARMS. See Section 4.6 for a detailed explanation.

Yellowknife Lake Study, 198	33 Data				
Identifier	#Iter	B(Ch1)	PBm	alphaB	Sum.Sq
		=====	====		=====
Station-01	28	5.7	0.55	1.49	0.010
Station 75 5-Jul-83	30	2.6	1.96	4.76	0.442

Fig. 4. Example cloudless solar PAR data generated by YPHOTO. These results were generated by the example presented in Section 4.7

Cloudle:	ss PAR	data	for 19	76 lat	itude	<b>= 50.0</b>	atmos.	_effect	t = 0.:	3250		
0.0	4.8	14.3	24.0	33.6	43.1	52.3	61.0	69.1	76.4	82.8	88.1	92.4
95.5	97.4	98.1	97.4	95.5	92.4	88.1	82.8	76.4	69.1	61.0	52.3	43.1
33.6	24.0	14.3	4.8	0.0	-1							
MAY 2												
0.0	5.3	14.8	24.4	34.1	43.6	52.7	61.4	69.4	76.7	83.1	88.5	92.7
95.9	97.7	98.4	97.7	95.9	92.7	88.5	83.1	76.7	69.4	61.4	52.7	43.6
34.1	24.4	14.8	5.3	0.0	-1							
MAY 3	•			•								
	5.8	15.2				53.1						
	98.0					88.8	83.4	77.1	69.8	61.8	53.1	44.0
34.5	24.9	15.2	5.8	0.0	-1							
MAY 4												
	6.2					53.5						
	98.3					89.1	83.7	77.4	70.1	62.1	53.5	44.4
	25.3	15.7	6.2	0.0	-1							
MAY 5								~				
0.0	6.7	16.1	25.7			53.9						
96.7		99.2			93.7	89.4	84.1	77.7	70.5	62.5	53.9	44.8
35.3	25.7	16.1	6.7	0.0	-1							
MAY 6	~ ~			05.7	45.4	54 A	40 Å	80 A	70.0			
	7.2	16.6				54.2						
97.0	98.9	99.5			93.9	89.7	84.4	78.0	70.8	62.8	54.2	45.1
35.7	26.2	16.6	7.2	0.0	-1							
MAY 7	7.6	17 A	06.6	26 1	45 5	EA C	62.0	<b>974 4</b>	70 1	04.7	00 0	04.0
	7.6 99.2					54.6 90.0				63.2		
36.1	26.6	17.0	7.6			30.0	04.1	10.3	11.1	03.2	54.0	45.5
MAY 8	20.0	17.0	1.0	0.0	-1							
0.0	8.1	17 /	27 0	36 5	4E Q	54.9	63 5	71 5	79 6	94 0	00.2	94.5
97.6						90.3						45.9
36.5	27.0	17.4		0.0		50.0	01.0			00.0	01.5	10.5
MAY 9	21.0	11.1	0.1	0.0	•							
0.0	8.5	17.9	27.4	36.9	46.2	55.3	63.8	71.8	78.9	85.2	90.5	94.7
97.8			99.7		94.7		85.2			63.8	55.3	46.2
36.9	27.4	17.9	8.5	0.0		50.0	00.2	, 0.5		00.0	00.0	10.2
MAY 10	#1 + Z	21.5	J. J	0.0	-							
0.0	8.9	18.3	27.8	37.3	46.6	55.6	64.2	72.1	79.2	85.5	90.8	95.0
98.1	99.9				95.0		85.5			64.2	55.6	46.6
37.3	27.8	18.3	8.9	0.0		55.5				~ * * * *	50.0	-0.0
		,		J. •	-							

Fig. 5. Example output from the program YPHOTO. These results were generated by the example presented in Section 4.7.

Lake Winn	ipeg	1976.	Cruise	3
-----------	------	-------	--------	---

								Depths					
-			0.00	1.20	2.40	3.60	4.80	6.00	7.20	8.40	9.60	10.80	12.00
		mg/m^2 -					mg C/	(m^3.d	ay)		~~~~		
MAY	1	163	28	27	26	24	19	1,3	7	4	2	1	0
MAY	2	328	56	54	52	47	38	25	15	8	4	1	0
MAY	3	494	84	82	78	71	58	38	23	12	6	2	0
MAY	4	662	113	110	104	95	78	51	30	16	8	3	0
MAY	5	831	142	137	131	120	98	65	38	20	9	3	0
MAY	6	1001	171	166	158	144	118	78	46	· 25	11	4	0
MAY	7	1173	200	194	185	169	138	92	54	29	13	5	0
MAY	8	1346	229	222	212	194	158	105	62	33	15	5	1
MAY	9	1519	258	250	239	219	179	119	70	38	18	6	1
MAY	10	1694	287	279	266	244	200	133	78	42	20	7	1
							<b>44382</b> 3		~ 4	*****			
tota	_	9.2	1.6	1.5	1.5	1.3	1.1	0.7	0.4	0.2	0.1	0.0	0.0
(gm	J					_							

INPUT DATA

Depths

0.00 1.20 2.40 3.60 4.80 6.00 7.20 8.40 9.60 10.80 12.00

PAR extinction: % of Surface PAR

MAY 5 100.00 57.54 33.11 19.05 10.96 6.31 3.63 2.09 1.20 0.69 0.40

Chlorophyll: mg/(m<sup>3</sup>)

alphaB: mg C/(mg chl.E.m^-2)

PBm: mg C/(mg chl.hr)

Command line: TESTYR

Solar data: Cloudless PAR data for 1976 latitude = 50.0 atmos\_effect = 0.3250

Warning: TESTYR, MAY 5: PAR extinction data extended to start date

Warning: TESTYR, JAN 1: alphaB data extended to finish date

Warning: TESTYR, DEC 31: PBm data extended to start date

Warning: TESTYR, MAY 5: PAR extinction data extended to finish date

Fig. 6. Example output from the program YTOTAL. These results were generated by the example presented in Section 4.8

### Lake Winnipeg 1976, Cruise 3

	4		<b></b>									
			Uncorr.		Morphometry						mean PAR	
			mg C/m2				mg C/m3		Mass Fixed, gm C		mE/m2.min	
		Depth	Total	Epi	Total	Epi	Total	Epi	To zmax	In Epi	Epi	Нуро
***									*******			33332
MAY	1	3.00	164	80	141	76	17	27	3.925E+08	2.098E+08	20.23	2.94
MAY	2	3.60	326	189	281	176	35	53	7.810E+08	4.901E+08	18.43	2.39
MAY	3	3.60	494	285	425	266	52	79	1.182E+09	7.391E+08	18.55	2.41
MAY	4	4.20	662	436	569	403	70	104	1.582E+09	1.120E+09	17.00	1.96
MAY	5	4.20	830	547	715	506	88	131	1.987E+09	1.406E+09	17.10	1.97
MAY	6	4.80	1003	735	863	673	106	154	2.398E+09	1.870E+09	15.77	1.60
MAY	7	4.80	1175	860	1011	788	124	180	2.808E+09	2.189E+09	15.86	1.61
MAY	.8	4.80	1345	986	1158	903	142	206	3.216E+09	2.508E+09	15.94	1.62
MAY	9	5.40	1521	1210	1308	1098	161	226	3.633E+09	3.049E+09	14.79	1.32
MAY	10	5.40	1696	1349	1458	1224	179	252	4.050E+09	3.399E+09	14.87	1.33
tota	als	(gm)	9.2	6.7	7.9	6.1	1.0	1.4	2.203E+10	1.698E+10		

Mean PAR values are calculated for 24 hour period

Maximum depth = 12.00

Number of depth intervals = 41

Command line: TESTYR, I=41

Cloudless PAR data for 1976 latitude = 50.0 atmos\_effect = 0.3250

Warning: TESTYR, MAY 5: PAR extinction data extended to start date Warning: TESTYR, MAY 5: PAR extinction data extended to finish date

Fig. 7. Example output from the program DPHOTO. These results were generated by the example presented in Section 4.9

Lake Winnipeg 1976, Cruise 3

Command line: TESTDAY

L. Wpg, Sta 318, 1976 Cloudless weather

INPUT DATA

PAR extinction: % of Surface PAR

JUN 6 100.00 56.37 31.78 17.91 10.10 5.69 3.21 1.81 1.02 0.57 0.32

Chlorophyll: mg/(m<sup>3</sup>)

alphaB: mg C/(mg chl.E.m^-2)

PBm: mg C/(mg chl.hr)

Warning: 318, JUN 6: Solar data missing; 70% of simulated cloudless used

Fig. 8. Example output from the program DTOTAL. These results were generated by the example presented in Section 4.10

Command line: TESTDAY, I=41
Lake Winnipeg 1976, Cruise 3

L. Wpg, Sta 318, 1976 Cloudless weather

Mean PAR values are calculated for 24 hour period

Maximum depth = 10.00

Number of depth intervals = 41