Daily Water Column Production (dwcpn)
[DRAFT] Software Manual

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Chapter 1

Introduction

This document provides information needed to use the `dwcpn` program.

1.1 Synopsis

`dwcpn [filename]`

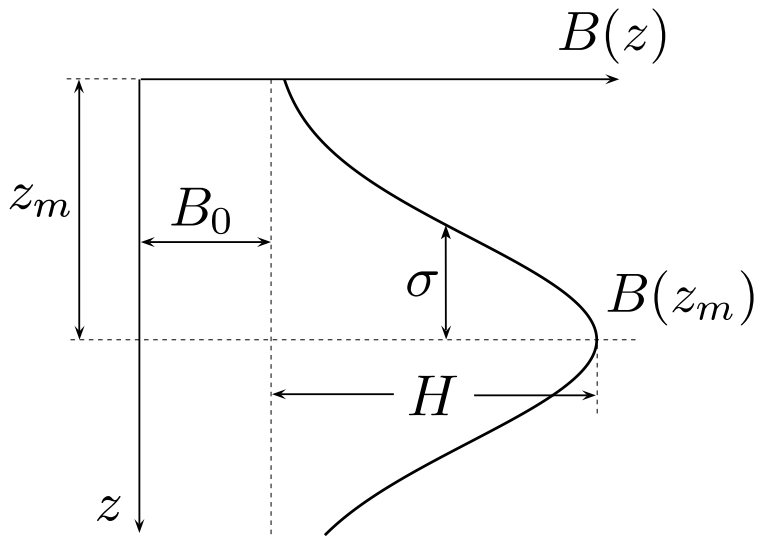
If the name of a suitable data file (extension "`.dat`" for Fortran format, "`.csv`" for comma-separated format) is provided, the program will run in "batch" mode and will create two new files (overwriting any existing files of the same name). The names of the new files are obtained by first removing any extension to obtain the "basename". The program will read data from "`basename.dat`", and will write the results on "`basename.out`". A processing log will be written on "`basename.log`".

1.2 Purpose

This program calculates estimates of daily, water-column production by numerical integration of a spectral model.

1.3 Description

This program computes the total daily, water-column production as described below (see Theory). The chlorophyll profile is modelled by a shifted-Gaussian curve (Figure 1.1), as described in Platt *et al.* (1994). Direct and diffuse components of



$$H = \frac{h}{\sigma\sqrt{2\pi}}$$

Figure 1.1: Shifted-Gaussian model for biomass–depth profile, $B(z)$.

the surface irradiance are computed using the clear sky, spectral irradiance model of Bird (1984), as adapted by Sathyendranath and Platt (1988), to give the spectral downwelling irradiance $I_0(\lambda, t)$ (Watts·m^{-2}) at the surface for a given location and zenith angle.

For each input data record, the program computes day length, D, surface irradiance, $I_0(\lambda, t)$, for 13 equally-spaced time steps from dawn to noon and 61 wavebands. An estimate for primary production is computed at each time step by integrating from the surface to the photic depth, and over wavelength. Total daily production is obtained by integrating from dawn to noon and doubling the result.

For large-scale calculations involving more than a few hundred records, it is generally more efficient to create input files and run the program in batch mode. For small calculations the R Ocean Production Extensions (ROPE) package allows the user to create a data frame for the input data and generate a new data frame

containing the results.

1.4 Input

The input data file consists of a two-line header followed by one or more data records. Each data record consists of values for location (latitude and longitude), the day number, photosynthesis–light parameters (α^B and P_m^B), and biomass parameters (z_m, B_0, h, and σ). A minimal example data file is:

```
Latitude Longitude Day alphaB  P_mB   z_m   B_0       h    sigma
(f6.2,x,f11.2,x,i3,x,f6.4,x,f6.2,x,f6.2,x,f7.5,x,f6.2,x,f6.2)
 30.00      -60.00  15 0.1060   3.67  74.70 0.08600  43.00  56.30
```

A recent addition made possible by the current Fortran standard is support for comma-separated value (CSV) format, indicated by the special format "`(*)`".

The fields in each input data record are as follows:

latitude (decimal degrees, −90° at the South pole to +90° at the North pole), format `fw.p`;

longitude (decimal degrees), format `fw.p`, although not required for the production calculations, is often useful in subsequent processing;

day number integer running from 1 to 365, format `iw`;

α^B the initial slope of the photosynthesis–light curve (mg C (mg Chl)$^{-1}$ h^{-1} (W m^{-2})$^{-1}$), format `fw.p`;

P_m^B the assimilation number (mg C (mg Chl)$^{-1}$ h^{-1}), format `fw.p`;

z_m "depth[1]" of the chlorophyll maximum, $-999.999 \le z_m \le 9999.999$ (m), format `fw.p`;

$B - 0$ the background component, $0 \le B_0 \le 9999.999$ (mg Chl m^{-3}), format `fw.p`;

h height parameter for the Gaussian component, $0 \le h \le 9999.999$ (mg Chl m^{-2}), format `fw.p`; and

σ Gaussian scale parameter, $0.001 \le \sigma \le 9999.999$ (m), format `fw.p`.

[1] In rare cases the fitting procedure will yield a negative estimate for z_m, *e.g.*, for two of the 28 cases shown in Table 3 of Platt *et al.* (1991), representing only three profiles in a data set of more than 600 profiles.

1.5 Output

When using Fortran format input files, the output file also consists of a two-line header followed by one output data record for each input record. For comma-separated input, the header consists of a single line with commas separating the column names. The output file corresponding to the above example is:

```
Latitude Longitude Day status   D     I_T   P_ZT
(f6.2,4x,f7.2,2x,i3,5x,i2,x,f5.2,x,f6.1,x,f7.1)
 30.00     -60.00   15      0 10.27 1643.4   255.0
```

The corresponding log file is:

```
Daily water-column production -- numerical integration of spectral model

Program: \PROJECTS\SOFTWARE\TEST\BIN\DWCPN.EXE
 Output file: dwcpn.out
 Log file:    dwcpn.log
 Input file:  dwcpn.dat

Limits:
  Value of epsilon in test (Daylength > epsilon):    .10000E-05
  Maximum depth (m):    250.50
  Depth increment (m):    .50000

Messages:

Summary:
     3 records processed (including two header records)
No processing errors.
```

The first two output records form the output data header, and are followed by one or more output data records. By convention, the first output record lists the output column names. When using legacy Fortran formatting, the second output record provides the Fortran format statement required to read the remaining output (data) records.

The fields in each output data record are as follows:

latitude (decimal degrees, -90° at the South pole to $+90^{\circ}$ at the North pole);

longitude (decimal degrees), although not required for the production calculations, is often useful in subsequent processing;

day number an integer running from 1 to 365;

status code (a status of 0 indicates no error, see Diagnostics for other codes);

day length D (h);

I_T total daily surface irradiance, (Watts $m^{-2}d^{-1}$); and

$P_{Z,T}$ daily, water-column production (mg C m^{-2}).

The first 3 values are simply copied from the input file.

1.6 Theory

[this space reserved for future additions]

1.7 Processing

The input data records are processed in a loop that reads one input data record, processes the data, and writes the corresponding output record. The longitude is not used in the calculations, but is stored as a double precision value and reproduced unchanged in the output data record.

1.8 Special cases

Two cases require special handling: a) the case where the noon zenith angle exceeds 80˚, and b) the case of twenty-four hour darkness (*i.e.*, day-length is zero). In the latter case, total daily production, $P_{Z,T}$, and total irradiance, I_T, are set to zero. In the case where day-length is not zero but the noon zenith angle exceeds 80˚, the values of $P_{Z,T}$ and I_T are set to missing value codes. In both cases, the status code is set to a positive value (see Diagnostics).

1.9 Files

In addition to the binary executable program and optical parameter file, one input data file is required. Two new files will be created, an output data file and a log file containing a record of the processing (previously existing files having the same names will be destroyed without warning). Each file is identified by its extension (the three letters following the "`.`" character):

1. the program (executable) itself (`.exe` extension on Windows);
2. optical parameters, `sam_penguin_globpars.inp`, from the directory given by the `OPHOME` environment variable;
3. input data (ASCII text, `.dat` extension);
4. processing log (ASCII text, `.log` extension); and
5. output data (ASCII text, `.out` extension).

With the exception of the optical parameters, file names are determined from the command line arguments at run time (*i.e.*, the program does not rely on any "hard-coded" data file names). When no file name is given on the command line, the program prints a usage message.

1.10 Requirements

The numerical calculations are time consuming but not otherwise demanding. An effort has been made to ensure that the results will remain consistent across a range of hardware platforms. It is assumed that double precision variables conform to the IEEE floating point arithmetic standard. This is the most efficient data type for floating point computations on modern microprocessors with hardware floating point support.

1.11 Bugs

Checks for missing or invalid input data are not exhaustive. In some cases it may be necessary to provide "cleaned" data to the program.

The software cannot easily be revised to allow computation of production in an arbitrary layer.

1.12 Limits

The maximum depth, depth increment used in the numerical integration, and the value of *epsilon* are shown in the log file.

1.13 Diagnostics

The following messages may occur:

This warning will be issued when the value for $I_0(t)$ cannot be determined at noon. The output status will be set to 1 and the remaining output variables will be given negative values.

This warning will be issued when the day-length is zero. The output status will be set to 2 and the remaining output variables will be given values of zero.

This warning will be issued when the computed zenith angle at noon is less than zero. The output status will be set to 5 and the output variables which cannot be computed will be given negative values. The value for day-length, D, will, however, be provided.

This warning will be issued when the the computed zenith angle at noon exceeds 80°. The output status will be set to 6 and the remaining output variables will be given negative values.

An error occurred in the `get_files` subroutine. This message will be preceeded by a message indicating the type of error that occurred.

An error occurred while reading or writing a file. This could indicate a missing or corrupted file, a disk problem such as lack of space, or a program which uses more files than the operating system configuration allows (many systems limit the number of files a program can use; in some cases the user may be able to increase this number via a configuration option).

The system function used to obtain the command line parameters returned an error. This may indicate lack of memory, an incompatible command processor, or a command line that is too long.

A program or file name was too long.

This is an internal program error which should not occur. The list of input file extensions passed to the subroutine has more entries than the number of files requested.

This is an internal program error which should not occur. The list of output file extensions passed to the subroutine has more entries than the

number of files requested.

The indicated file could not be opened. The file name may have been entered incorrectly or the file may have a hidden, read-only, or system attribute.

An error occurred while reading from or writing to a file or the console. This could indicate a missing or corrupted file, a disk problem such as lack of space, a buffer overflow, or a control character inadvertently entered from the keyboard.

This is not always an error, but may indicate a file that has been truncated or damaged.

A problem occurred with an input file. The file name passed to the program may be incorrect, or the file may have a hidden or system attribute.

A problem occurred with an output file. The file name passed to the program may be incorrect or the file may have a hidden, system, or read-only attribute.

The input record format (obtained from the second line of the input file) did not have the required number and types of fields.

Chapter 2

Installation and configuration

This chapter describes the steps needed to compile and run the daily water column production program, `dwcpn`.

It is impossible to provide binary versions that work on all systems, and many applications will require changes to the program to adapt to the available input data or customize the output.

In order to use the program, most users will need to compile a version that runs on their system.

An outline of the process is:

Verify that the development tools are properly installed

- create a small example
- build the example using make
- run the example

Configure the build system

- directories
- `Makefile`

Build the program

- build and install the library
- build and install the program
- run the program

Chapter 3

Obtaining development tools

Linux users should be able to install suitable tools using the package manager for their linux distribution. Windows and Apple users will have to install 3rd party software. A number of vendors offer high quality Fortran 95 compilers for Windows, and there are also many ways to obtain open source tools. Apple Mac OS X users will have to install Apple's Development packages and then obtain a fortran compiler.

3.1 Linux

Most linux distributions provide GNU `gfortran`. Versions 4.2 and higher should be suitable.

For some older distributions, the version of gfortran available from the distribution may not work well. Alternatives include commercial compilers from Intel and Sun, and the free g95 compiler.

In general, binaries generated on somewhat older versions of linux run on newer versions. To produce binaries for others to use, an older version of linux should be used. This may present difficulties if the hardware is not supported by the older linux version. One solution is to install a minimal configuration in a virtual machine running under windows or a more recent version of linux.

3.2 Windows

Commercial compilers are sold by a number of vendors, including Intel. Free compilers include both gfortran and g95.

If you plan to use free compilers, the simplest approach is to install Octave, which includes a complete set of GNU compilers used to build Octave and user-installable packages. It will be necessary to adjust the user PATH setting to make these compilers available in the cmd shell.

3.3 Apple Mac OS X

Apple does not provide a Fortran compiler. Commercial compilers are available from Intel. Free compilers include gfortran and g95. Apple's Xcode development packages must be installed. A version is provided on the install DVD, but in most cases users should register with Apple as developers and obtain the current version of Xcode.

3.4 Unix

Most unix systems provide compilers, but Fortran 95 compilers may not be available for older systems. In many cases it is possible to build current versions of gfortran or g95.

3.5 Checking the build system

3.6 Checking the program

Once you have compiled `dwcpn` you should run it on a small data file and check that the results match those obtained previously. The `ndiff` program is useful for comparing output files when there are differences in formatting resulting from using different compilers and libraries or from numerical round-off errors.

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Notation

α^B	initial slope of relationship between photosynthesis and irradiance, $\alpha^B \equiv \partial P^B/\partial I|_{I\to 0}$, mg C (mg Chl)$^{-1}$ h^{-1}(W m^{-2})$^{-1}$.
$\alpha^B(\lambda)$	photosynthetic action spectrum, mg C (mg Chl)$^{-1}$(W m^{-2})$^{-1}$ nm^{-1}.
B	biomass, as concentration of Chlorophyll a, mg Chl m^{-3}.
$B(z)$	chlorophyll concentration as a function of depth, mg Chl m^{-3}.
B_0	background concentration in the shifted-Gaussian model, mg Chl m^{-3}.
D	day-length, hours.
h	parameter for the amplitude of the chlorophyll maximum in the shifted-Gaussian model, mg Chl m^{-2}.
$I_0(\lambda, t)$	downwelling irradiance at the surface, Watts·m^{-2}·nm^{-1}.
$I(z, \lambda, t)$	available light at depth z.
I_T	total irradiance at the surface, Watts· m^{-2}d^{-1}.
$\Pi(z, \lambda, t)$	rate of photosynthesis, mg C (mg Chl)$^{-1}$ h^{-1}(nm)$^{-1}$.
$P_{Z,T}$	daily water-column primary production, mg C m^{-2}.
P_m^B	assimilation number, specific production at saturating light, in the absence of photoinhibition, $P_m^B = P^B|_{I\to\infty}$, mg C (mg Chl)$^{-1}$ h^{-1}.
σ	scale parameter for the width of the peak in the shifted-Gaussian model, m.
z	depth (origin at surface, positive downwards), m.
z_m	"depth" (in rare cases, the value of z_m may be negative) of chlorophyll maximum, in the shifted-Gaussian model, m.

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