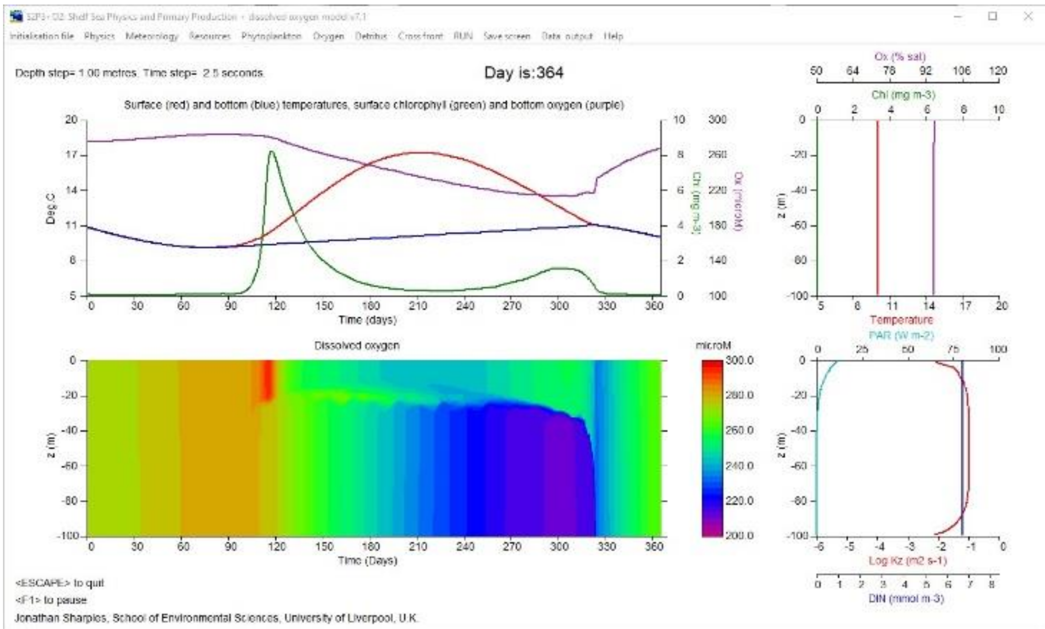
Guide to the S2P3+O2 Model



Jonathan Sharples

School of Environmental Sciences

University of Liverpool

UK

Contents:

1. Introduction

This 1-D (vertical) model is designed for use as an investigative and educative tool for problems concerning the link between the physical structure of the water column and primary biological production in coastal and shelf seas.

The physical model is forced by tidal currents, wind stress, and surface heat flux (solar radiation and surface heating/cooling). A turbulence closure sub-model provides the important link between vertical turbulent transfers of scalars and water stability. The biological component of the model is a simple cell quota model of carbon fixation, with one species of phytoplankton growing in response to light and dissolved inorganic nitrogen.

This model is an updated version of the S2P3 model published in Simpson & Sharples, *An Introduction to the Physical and Biological Oceanography of Shelf Seas*, CUP, 2012. The main difference is that S2P3+O2 includes simulation of dissolved oxygen in the water column. This includes the roles of respiration, organic matter production and remineralisation, and the air-sea flux of oxygen between the sea surface and the atmosphere.

A second difference between this new version and the original S2P3 v7.0 model is that the meteorological forcing now uses hourly data, rather than daily means. This was done because of the availability of the ERA5 meteorological data product from the European Centre for Medium Range Weather Forecasting (ECMWF). See the section on Meteorology for more details.

The user has control over all model physical and biological driving parameters. Graphical screen output, suitable for basic visualisation and teaching, is generated as the model operates. More detailed data is written to files for later analysis.

The physics equations used by the model are detailed in:
Sharples, J., et al., *Continental Shelf Research*, **26**, 733-751, 2006.

A full description of the biological model (not including the oxygen components) can be found in:
Sharples, J., *Journal of Plankton Research*, **30**, 193-197, 2008.

A description of how the model processes oxygen is included in this document.

The model has been written in Fortran (compiled using Lahey LF95 v7.3, www.lahey.com) and uses the *Winteracter* Fortran GUI toolset (Interactive Software Services Ltd., www.winteracter.com).

The model is supplied as an executable application that will only run under the Windows operating system.

This manual repeats the material available within the model Help, along with a section below providing basic instructions to get the model running.

2. Getting Started

Two files are required:

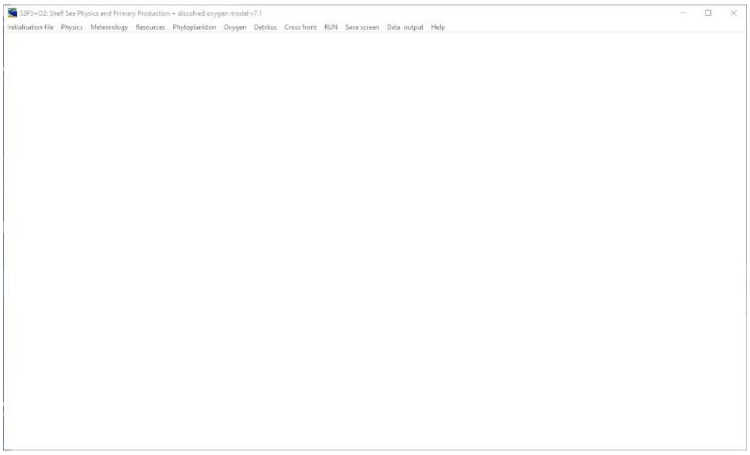
S2P3_O2.EXE	The model application
S2P3_O2_MODEL.CHM	Help and instructions, called by the model help/instructions links

Note that the model will still run without the help file; instead you can refer to this document for advice on the model.

Create a folder on your computer's hard drive (e.g. c:\S2P3O2) and put the above files into it.

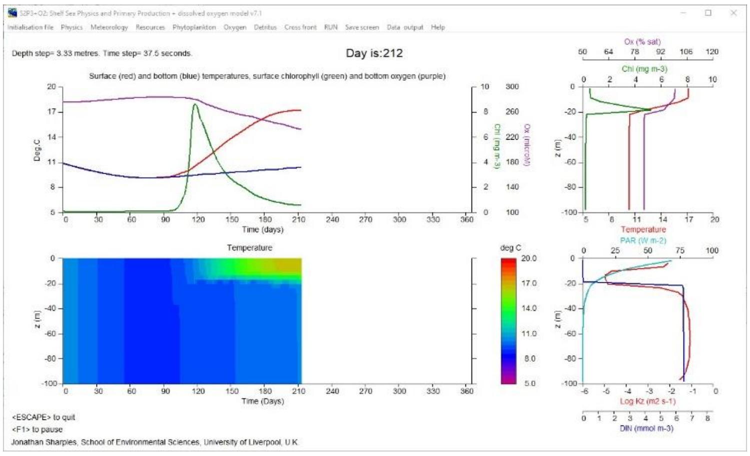
Within Windows Explorer, go to your model directory and double-click the model icon:

The main model window then opens:



If you now click on the RUN option in the main menu, the model will run through one year of the default set-up. This default run is for conditions similar to the central Celtic Sea on the NW European shelf (51° N, 8° W), with seasonally-smoothed meteorological forcing (see **Meteorology** below).

During the model operation the screen output looks like:

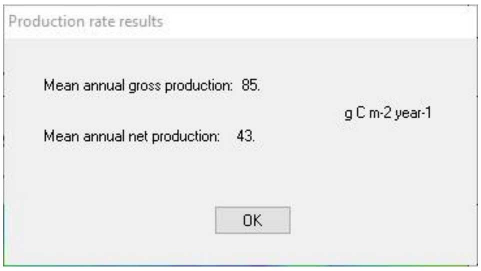


As the model runs, data is output to the plots on the screen once per day, at noon. The plots to the left of the screen are time series, starting on January 1st and running through to December 31st. The upper plot on the left shows time series of the surface (red) and near-bed (blue) temperatures (°C), the surface chlorophyll concentration (green line, mg m^{-3}) and the near-bed concentration of dissolved oxygen (purple line, µM). The lower left plot illustrates the time series of the vertical structure of one of temperature (^{o}C), phytoplankton biomass (mg chl m^{-3}), dissolved oxygen (µM) or the vertical eddy diffusivity (m^2 s^{-1}) as coloured contours: the choice of which variable to contour is selected in the **Data output** menu. You can see in the above example how the default model run generates a seasonally-stratifying water column, with a spring phytoplankton bloom (see Simpson & Sharples, 2012, Chapter 6) and summer phytoplankton biomass located along the thermocline (see Simpson & Sharples, 2012, Chapter 7).

The plots to the right are vertical profiles of modelled parameters, refreshed at noon each day. Upper right plots show temperature (red, °C), chlorophyll concentration (green, mg m^{-3}), and dissolved oxygen saturation (purple, %). The lower right plots show profiles of dissolved inorganic nitrogen concentration (dark blue, mmol m^{-3}), the vertical distribution of daily-mean photosynthetically active radiation (light blue, W m^{-2}), and $\log_{10}$ of the daily-mean vertical diffusivity (red, m^2 s^{-1}).

While the model is running you can pause it by pressing the F1 key on the keyboard. Resume the run by selecting OK as prompted. The model can be stopped at any point by pressing the keyboard

<escape> key. When the model ends, either at the end of a year's simulation or following <escape>, a summary of the annual primary production is reported:



Now that you have got the model running, the details of the menu options and how you can alter the physical and biological parameters that control the results are described below.

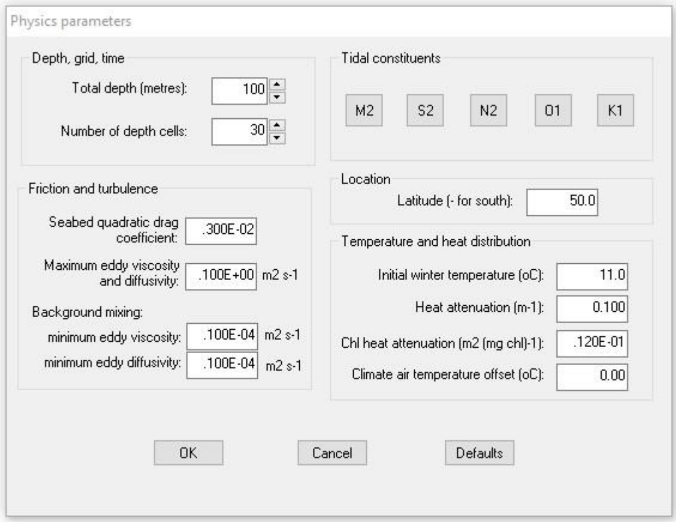
3. Model Operation: Dialogs for controlling model parameters.
The model requires a set of initial parameters that describe the physical environment, the characteristics of the primary producers and how organic material is remineralised. There are also some output parameters that can be altered, both for the graphical display and for the data output by the model. All parameter input dialogs have a "default" option. Selecting this restores the default values to all parameters *within that dialog*.

3.1 ***Initialisation file:*** *Saving or loading parameter sets.*
The initialisation parameters that are set up in the model menus can be saved into a text file, and later re-loaded to run the model again with the same parameters. You can have a look at the parameters in the initialisation file by running the model application and clicking on **Initialisation file** and **Save**. In the *Save initialisation parameters* dialog supply a file name (*.txt) and click Save.

The initialisation file is written in standard ascii text which can be viewed using your favourite editor (e.g. Microsoft Notepad works well). Try to avoid viewing the initialisation file with anything that might upset the formatting. The model requires the initialisation file to have the correct format, otherwise you might re-load incorrect parameters or crash the model. If the initialisation file does not exist, or if there is a formatting issue with the supplied initialisation file, then the model reports an error. In that case make sure that your initialisation file exists, and make sure it has the right format (e.g. run the model with all defaults and save a default initialisation file, then compare that file to the one that failed).

The model will attempt to run with any parameters that you supply, but obviously some will be more realistic than others. The following sections describe the parameters that can be selected from the menus, and that can be written to an initialisation file. I have included suggested sensible ranges for most parameters. Don't feel too inhibited in drifting out of these suggested ranges, but do make sure you think carefully about the numbers you are supplying and whether or not they are physically or biogeochemically reasonable.

*3.2 **Physics**: setting the main physical parameters.*



Total depth (metres): total water column depth, typically between 10 and 300 metres for a shelf sea.

Number of depth cells: this determines the model vertical resolution. Total depth divided by number of depth cells is the thickness of the individual depth cells used in the model grid, Δz (metres). More depth cells provide better resolution, but the model will run much slower. The maximum number of depth cells allowed is 200.

The thickness of the model grid cells is calculated by the model as (total depth/number of depth cells). The timestep, Δt , is calculated by the model based on Δz and the maximum allowable turbulent viscosity and diffusivity ($N_z^{\max}$) using a simple stability condition.

$$\Delta t < \frac{\Delta z^2}{2N_z^{\max}}$$

The time step needs to be small enough for the model to "see" something being mixed through a depth cell, otherwise the model will become unstable. The time step is proportional to the squared depth cell thickness, so if you double the number of depth cells (i.e. halve Δz) you will reduce the time step by a factor of 4. Generally, you might want to run the model with fairly coarse resolution (e.g. a depth cell thickness of 4 metres) initially to explore the results quickly. When you have decided what set of parameters you are particularly interested in, reduce the cell thickness to get better resolution in the model output.

Latitude (degrees): this is positive for the northern hemisphere, negative for the southern hemisphere (so a range of -90 deg to + 90 deg). Note in the original version of the S2P3 model the latitude was used to calculate the daily-mean clear sky solar short-wave radiation. This new version of the model takes the short-wave radiation from the meteorological data (see ***Meteorology*** below). The latitude is only used for calculation of the Coriolis parameter.

Bottom quadratic drag coefficient: this is the variable k_b in the book and controls the strength of bed friction. Typical values are 0.001 to 0.005.

Maximum diffusivity and viscosity ($m^2\ s^{-1}$): this provides some further control on the time step used by the model (see "Time step" above). In regions of the water column where there is convective instability (e.g. the sea surface when there is surface cooling) the turbulence closure scheme can generate large values for the vertical eddy viscosity and diffusivity. It is possible for maximum values to reach above 0.5 $m^2\ s^{-1}$. However, a value of 0.1 $m^2\ s^{-1}$ is usually sufficient to remove convective instabilities quickly, and constraining the model to this maximum helps keep the time step from getting too small. Reducing this constraint to below 0.05 $m^2\ s^{-1}$ is not advisable. It is always worth checking that limiting the turbulent mixing in this way does not have a serious effect on the model results. For instance, if the value is set too low you will see significant unstable temperature profiles persisting during winter.

Background viscosity ($m^2\ s^{-1}$): This is a simple way of incorporating the mixing effects of interior processes such as internal waves or natural variability in the meteorological forcing (see, for instance, Sharples & Tett, *Journal of Marine Research*, **52**, 219-238, 1994). The model cannot simulate these interior processes (see Chapter 7 of the book), but not allowing for the mixing generated by them can have important consequences for the physics and the biogeochemistry. Typical values for the weak internal waves in the central Celtic Sea might be 1×10^{-5} to 5×10^{-5} $m^2\ s^{-1}$, while approaching the stronger internal wave regime of the shelf edge could raise this by a factor of 10.

Background diffusivity ($m^2\ s^{-1}$): See "background viscosity" above.

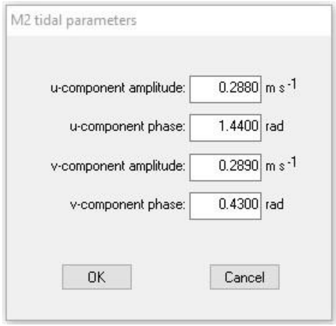
Initial water temperature (°C): The model starts the annual simulation on January 1st. In temperate northern hemisphere shelf seas the water column is usually well-mixed at this stage of winter, and this initial water temperature sets the modelled vertically-mixed water column temperature. Note that it is not the coldest temperature that the water column will reach; cooling could continue into early spring. If you are not sure what the initial water temperature in winter might be, estimate it and see what temperature the model predicts at the end of the year simulation. You can then use this prediction as your initial temperature - a few iterations of this might be necessary to get the initial temperature set correctly. For the southern hemisphere you need to assume that the first day of the annual simulation is 1st July and remember to configure any meteorological data to be consistent with this (see information on the **Meteorology** dialog below).

Heat vertical attenuation (m^{-1}): this is the attenuation coefficient that controls the exponential decay of heat down through the water column. A typical near-surface shelf sea value might be 0.1 m^{-1} in stratified regions, or as high as 0.4 m^{-1} in mixed regions where significant suspended material or CDOM limits heat transmission. The model applies a very simple approach to the wavelength dependence of radiation attenuation. The red end of the solar radiation spectrum is absorbed very rapidly, which is simulated by dumping 55% of the incident radiation into the top grid cell. The remaining 45% of the radiation is distributed exponentially using the heat vertical attenuation coefficient.

Chl effect on heat attenuation (m^2 (mg Chl)$^{-1}$): this quantifies the effect of chlorophyll in the water raising the water opacity, and so affecting the attenuation of heat through the water. Note the units are equivalent to m^{-1} (mg Chl m^{-3})$^{-1}$, hence the impact is described in terms of a change in attenuation coefficient per unit of chlorophyll concentration. A typical value is 0.012 m^2 (mg Chl)$^{-1}$. See Kirk, J. T. O., *Light and Photosynthesis in Aquatic Ecosystems*, Cambridge University Press, 2010 for more details.

Climate air temperature offset (ºC): I added this into the model as it was useful for students working on investigations of how shelf seas might respond to a warmer climate. A warming climate affects the shallow shelf seas mainly through the change in temperature of the overlying atmosphere. This climate temperature offset is added to the air temperature data in the meteorological forcing, thus mimicking the effects of changes in the atmospheric temperature. Note that if you add a temperature offset, then the shelf sea will gradually warm up and the final winter temperature (December 31st) will be greater than the initial winter temperature (January 1st). Ideally the model would need to be run for 3 or so years in order that the water column reaches an equilibrium seasonal cycle with the new temperatures. You can do this either by iteratively changing the initial winter temperature based on the final temperature reached by the model, or you can get very close by adding the climate offset to the initial winter temperature used by the model.

*3.3 **Physics – tidal constituents:** tidal parameters set by the constituent buttons:*
Tidal constituent information required by the model is input by selecting the constituent from the Physics dialog:



u amplitude (m s^{-1}): the amplitude of the tidal current along the x-axis (east-west) for each of the 5 tidal constituents M2, S2, N2, O1 and K1.
u phase (radians): the phase of the tidal currents along the x-axis for the 5 tidal constituents.
v amplitude (m s^{-1}): the amplitude of the tidal current along the y-axis (north-south) for each of the 5 tidal constituents.
v phase (radians): the phase of the tidal currents along the y-axis for the 5 tidal constituents.

Tidal Forcing in the Model
The barotropic tidal flow in the model is generated by a sea surface slope (or horizontal pressure gradient) that oscillates at the tidal frequency. The 5 tidal constituents have periods:

M2 (principal lunar tide)	period = 12.42 hours
S2 (principal solar tide)	period = 12.00 hours
N2 (principal lunar elliptic)	period = 12.66 hours
O1 (principal declinational)	period = 25.82 hours
K1 (declinational)	period = 23.93 hours

Typically, you may have tidal constituent information based on *u* (east-west) and *v* (north-south) currents measured by a current meter. The data required by the model assumes that you have performed a harmonic analysis separately on the *u* and *v* current data recorded close to the sea surface, fitting the data to a tidal equation of the form:

$$u = A\cos\left(\omega_{tide}t - \phi\right)$$

where ω_{tide} is the frequency of the tidal constituent. Make sure that the units of ω_{tide} and time (t) are consistent, and if you want to attempt to get the timing of the tide close to your observations make sure that the time axis of your current data has t =0 at midnight on January 1st (i.e. the same as the model). *A* (m s^{-1}) is the amplitude of the tidal constituent and ϕ is the phase angle (radians) that sets the timing of the tidal currents. For each tidal constituent the model requires 2 values for *A* (one for the *u*-component and one of the *v*-component) and 2 values of ϕ.

The model uses this tidal constituent information and the Coriolis parameter, *f*, calculated from the latitude to calculate the pressure gradient amplitudes needed to generate a tidal current ellipse similar to the one which has characteristics resulting from your harmonic analysis. Using your tidal information, the model calculates the length of the semi-major axis of the tidal current ellipse (*S*), the polarisation of the ellipse (*P*), and the orientation of the major axis measured anti-clockwise from the x-axis. The pressure gradient amplitudes along the major and minor axes of the ellipse (PG_{major} and PG_{minor}) for a tidal constituent are then given by:

$$PG_{major} = S\left(\omega_{tide} + Pf\right)$$
$$PG_{\mathrm{minor}} = S\left(f + P\omega_{tide}\right)$$

The orientation of the tidal current ellipse is used to transform the pressure gradient into *x* and *y* components.

This calculation of the pressure gradients assumes that the surface currents that provided the tidal constituent information are largely free of frictional effects from the bottom boundary layer. In many cases this will be an approximation, so the resulting modelled tidal currents may differ from your observations. The differences occur mainly in the phasing of the currents. Ideally, if detailed knowledge of the modelled currents compared to your observations is required, you should use the hourly data output (see Data Output below) to generate some current data on which you can then perform a harmonic analysis and check the modelled currents against your observations.
Note that the constituent phase angles are relative to 0000 hrs January 1st on the year of the model simulation.

The default tidal parameters are based on harmonic analysis of currents measured by a mooring in the Celtic Sea deployed as a part of the UK Shelf Sea Biogeochemistry research programme. A full description of what was seen by the mooring can be found in *Wihsgott et al., Progress in Oceanography*, 177, 2019.

*3.4 **Meteorology**: setting the weather used by the model.*

Meteorological data requirements are different to those in the earlier S2P3 v7 model. The main difference is that the model now uses hourly data, rather than daily mean data. I have done this because of the availability of the ERA5 reanalysis product from ECMWF, which provides hourly meteorology data, globally with 0.25^o latitude and longitude resolution, from 1959 to the present.

The Meteorology dialog offers two choices for the meteorological data to be used by the model.

1. Default (Celtic Sea) meteorology.
This is a set of meteorology data based on a seasonal analysis of information from North Atlantic model of the UK Met Office. The 3-hourly data, from the meteorological model grid cell located at 50 deg N 7 deg W (central Celtic Sea), was averaged to daily values and then fitted to a sinusoidal curve with period 1 year. This yielded smooth functions describing the meteorological forcing parameters as a function of the annual cycle (yearly angular frequency ω) and time, t. The functions used are:

$$\text{wind speed} = \sqrt{62.9 + 26.8\cos(\omega t) + 7.9\sin(\omega t)} \quad [\text{m s}^{-1}]$$
$$\text{air temperature} = 12.5 - 3.3\cos(\omega t) - 2.5\sin(\omega t) \quad [^{\circ}\text{C}]$$
$$\text{air pressure} = 1016 \times \left(1.014 - 0.0004\cos(\omega t) + 0.0009\sin(\omega t)\right) \quad [\text{mbar}]$$
$$\text{relative humidity} = 81.4 - 2.3\cos(\omega t) + 0.8\sin(\omega t) \quad [\%]$$
$$\text{cloud cover} = 66.5 + 5.1\cos(\omega t) - 4.1\sin(\omega t) \quad [\%]$$

Wind direction simply rotates by +72 degrees each day, and the x- and y-components of the wind speed calculated. The S2P3+O2 model uses meteorological data with 1-hour resolution. The meteorological variables above are calculated with this resolution. For the surface short wave radiation, the clear sky mean daily radiation (W m^{-2}) and clear sky noon radiation (W m^{-2}) for each day of the year (j) are calculated from:

$$\text{mean daily short wave radiation}(j) = 195.0 - 144.9\cos(0.172j) + 30.9\sin(0.172j) \quad [\text{W m}^{-2}]$$
$$\text{noon short wave radiation}(j) = 606.7 - 316.9\cos(0.172j) + 70.8\sin(0.172j) \quad [\text{W m}^{-2}]$$

and the day length (in hours) is calculated for each day of the year by:

$$\text{day length}(j) = 12.2 - 3.94\cos(0.172t) + 0.69\sin(0.172t) \quad \text{[hours]}$$

with 0.0172 radians per day as the annual cycle frequency.

Hourly radiation during a day is then calculated as having cosine variability, centred on noon with the clear sky noon radiation, with daylight hours +/- 0.5*day length either side of noon. A check is made to ensure the resulting mean daily radiation is the same as that calculated above. Finally, the cloud cover (c , %) is used to reduce the surface radiation via:

$$\text{radiation (with cloud)} = \text{clear sky radiation} \times \left(1.0 - 0.004c - 0.000038c^2\right)$$

Each time the model is run with these default functions, a file "default_met.dat" is written containing the hourly meteorological data with the following columns:

> time (days), wind velocity x-component (m s^{-1}), wind velocity y-component (m s^{-1}), air temperature (^{o}C), air pressure (mbar), relative humidity (%), radiation (W m^{-2}), cloud cover (%)

This default file can be useful. For instance, you could edit the file to have one strong wind event in summer to investigate what happens when a single storm passes through a shelf sea. The file has the format needed to load back into the model (see *User defined meteorology* below).

2. User defined meteorology.
You can supply your own meteorological forcing by setting up an ascii text file with hourly meteorological data with columns:

> time (days), wind velocity x-component (m s^{-1}), wind velocity y-component (m s^{-1}), air temperature (^{o}C), air pressure (mbar), relative humidity (%), radiation (W m^{-2}), cloud cover (%)

For an example of the required file format, see the file "default_met.dat" generated by the model when run with the default Celtic Sea annual cycles.

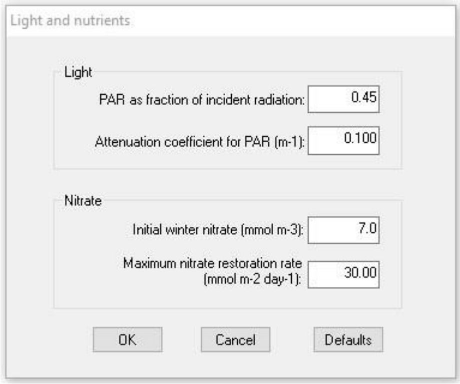
Use the Browse button in the Meteorology dialog to select the file containing your meteorology data. The model will report back if it finds that it cannot read the format of the file.

Note that if extracting ERA5 data to generate meteorological data files for the model, the relevant ERA5 variables to download are:

> u10, v10: x- and y-components of the 10-metre wind velocity [m s^{-1}]
> d2m: dewpoint temperature at 2 metres [degrees K]
> t2m: air temperature at 2 metres [degrees K]
> msl: sea level air pressure [Pa]
> ssrd: surface solar radiation [J m^{-2}]
> tcc: total cloud cover [fraction]

Relative humidity can be calculated from the dewpoint and air temperatures. Note the units for the ERA5 variables, which in some cases will need to be converted for the model meteorological forcing.

3.5 ***Resources****: controlling light and nutrient.*



PAR attenuation coefficient (m^{-1}): similar to the heat vertical attenuation (see above), but here specific to the wavelengths of light that form PAR. A typical value in clear shelf waters is 0.1 m^{-1}, but increasing to 0.4 m^{-1} or higher in turbid regions.

Fraction of surface radiation that is PAR: The model is forced by total radiation at the sea surface, supplied in the meteorological data. Typically, about 45% of that total radiation (i.e. a fraction 0.45) is within the range of wavelengths that make up PAR.

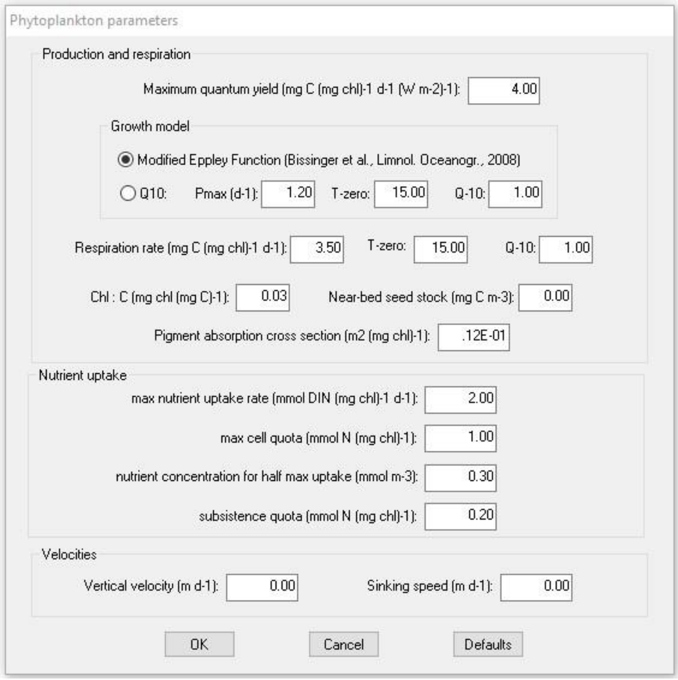
Initial winter nitrate (mmol m^{-3}): all grid cells in the model vertical profile are initialised to this concentration of dissolved inorganic nitrogen (DIN) at the start of the modelled year. A typical mid-Celtic Sea value is 7 - 9 mmol m^{-3}.

Maximum nitrate restoration rate (mmol m^{-2} d^{-1}): the model is not 100% efficient at returning organic nitrogen back to inorganic nitrogen (on the timescale of a few years a real shelf sea probably is not either). In reality shelf sea nitrate will be maintained, over a long time scale, by processes such as benthic remineralisation, ocean-shelf transfers and estuarine inputs. The model includes a benthic flux of nitrate into the bottom grid cell (which we can think of as a combination of nitrogen remineralised by the benthos and deep water transport from the ocean). At each time step, the updated nitrate concentration in the bottom grid cell, DIN_{new} (mmol m^{-3}), is calculated as:

$$DIN_{new} = DIN_{old} + \left(\frac{N_{rate}}{24 \times 3600}\right)\left(1 - \frac{DIN_{old}}{DIN_{winter}}\right)\frac{\Delta t}{\Delta z}$$

where DIN_{old} (mmol m^{-3}) is the old nitrate concentration in the bottom grid cell, N_{rate} is the maximum nitrate restoration rate (mmol m^{-2} day^{-1}), DIN_{winter} (mmol m^{-3}) is the initial winter nitrate concentration, Δt (seconds) is the model time step and Δz (metres) is the grid cell thickness. The default value of N_{rate} = 30 mmol m^{-2} day^{-1} is set simply to return the winter nitrate back to DIN_{winter} by the end of the year. This benthic input is only applied if $DIN_{old} < DIN_{winter}$, which allows for the possibility of DIN in the bottom water increasing above DIN_{winter} if, for instance, a large supply of organic nitrogen to bottom waters is remineralised in stratified conditions.

3.6 ***Phytoplankton – Growth****: controlling photosynthesis and nutrient uptake.*



Max quantum yield (mg C (mg Chl)$^{-1}$ d^{-1} (W m^{-2})$^{-1}$): this is the parameter α_q in the PAR-growth curve (see Simpson & Sharples, 2012, Chapter 5). It controls the initial slope of the curve as light increases from zero. The model default is 4.0 mg C (mg Chl) d^{-1} (W m^{-2})$^{-1}$. A useful range is between about 1 and 10 mg C (mg Chl) d^{-1} (W m^{-2})$^{-1}$.

Growth model: this sets which formulation for phytoplankton growth to use. Selecting the Modified Eppley Function option in the dialog tells the model to use a relation between maximum phytoplankton growth rate and temperature (see: Bissinger et al., *Limnology & Oceanography*, 53(2), 487-493, 2008):

$$P_{\max}^{b} = 0.81e^{0.0631T} \quad [\text{d}^{-1}]$$

Note that $P_{\max}^{b}$ is the maximum growth rate (e.g. g C m^{-3} d^{-1} or g Chl m^{-3} d^{-1}) normalised by biomass concentration in the same units (e.g. g C m^{-3} or g Chl m^{-3}). This growth rate, the associated biomass, and the temperature, T , are those at the grid cell in the model at which growth rate is being calculated.

Selecting the Q10 option in the dialog tells the model to use a Q_{10} description of phytoplankton growth as a function of temperature. The Q_{10} description (see for instance Valiela, I., *Marine Ecological Processes*, Springer, 2010) describes the temperature dependence of some biological rate, *r*, as:

$$Q_{10} = \left(\frac{r_1}{r_2}\right)^{10/(T_1 - T_2)}$$

with rate r_1 measured at temperature T_1 and r_2 at T_2. Most biological rates have Q_{10} between 2 and 3. The rate, r , at some temperature T is then:

$$r = r_2 Q_{10}^{\,(T - T_2)/10}$$

This parameterisation of growth rate requires 3 parameters to be specified:

Reference maximum growth rate (d^{-1}): this is a biomass normalised growth rate, e.g. r_2 (d^{-1}) in the equation above, and will be the maximum that the phytoplankton can achieve (i.e. neither light nor nutrients limiting) at the reference temperature, T_2, of the Q_{10} formulation. It is a time scale for doubling phytoplankton biomass. A typical value might be about 1 d^{-1}, with a sensible range between about 0.25 and 2 d^{-1}.

Reference temperature (°C): the reference temperature, T_2, at which the maximum growth rate is that above. The Q_{10} formulation will raise growth rate when the temperature is above the reference temperature and reduce growth rate below the reference temperature.

Q_{10} exponent for growth: this controls the sensitivity of the growth rate temperature dependence, with higher exponents leading to greater changes to growth with temperature. A typical value for phytoplankton is 2. If the exponent is set to 1 (the default value) then there is no temperature dependence and the maximum growth rate is always the reference maximum growth rate.

Note that the above 3 parameters only appear in an initialisation file if the growth model has been set to 2.

Reference respiration rate (mg C (mg Chl)$^{-1}$ d^{-1}): phytoplankton respiration is described using a Q_{10} formulation (see the above description of the growth model). The reference respiration rate is that measured at some reference temperature (see below). The model default is 3.5 mg C (mg Chl)$^{-1}$ d^{-1}. A suitable range is difficult to define, and measurements are harder to find than those of growth rate.

Reference temperature for respiration rate (°C): the temperature at which the reference respiration rate (above) was measured.

Q_{10} exponent for respiration: this controls the sensitivity of the respiration rate temperature dependence, with higher exponents leading to greater changes to respiration with temperature. Typical values for phytoplankton are between 2 and 3. If the exponent is set to 1 (the default value) then there is no temperature dependence and the respiration rate is always the reference rate.

Chl:carbon (mg Chl (mg C)$^{-1}$): the amount of chlorophyll in the phytoplankton per unit of carbon. Typically, we expect this value to change, both between species in a community and within one species as the light it receives varies. The use of a single, fixed value is an important assumption made by the model. Typical values have been measured at 0.01 - 0.05 (Holligan et al., *Marine Ecology Progress Series*, **14**, 111-127, 1984), with higher values generally associated with phytoplankton at the thermocline.

Near-bed seed stock (mg C m^{-3}): this can be used to prevent a phytoplankton species from completely disappearing, or perhaps to simulate the over-wintering of phytoplankton cysts. The model prevents the bottom depth cell phytoplankton concentration from dropping below this seed value. The default value is 0 mg C m^{-3} (i.e. seed stock not used).

Pigment absorption cross-section (m^2 (mg Chl)$^{-1}$): the effect of phytoplankton biomass on the absorption of light (PAR) through the water column. Default value is 0.012 m^2 (mg Chl)$^{-1}$. See Kirk, J. T. O., *Light and Photosynthesis in Aquatic Ecosystems*, Cambridge University Press, 2010 for more details.

Maximum nitrate uptake rate (mmol (mg Chl)$^{-1}$ d^{-1}): the maximum rate at which phytoplankton can assimilate nitrate from the surrounding pool of inorganic nitrogen. It is the value that the Michaelis-Menton uptake curve approaches at high ambient inorganic nitrogen (see Simpson & Sharples, 2012, Chapter 5). The default value is 2 mmol (mg Chl)$^{-1}$ d^{-1}. Model results are not overly sensitive to this value, unless it is changed by a factor of 10, as nitrate assimilation is strongly inhibited by the phytoplankton reaching the maximum cell nutrient quota (see below).

Maximum cell nutrient quota (mmol N (mg Chl)$^{-1}$): the maximum amount of nitrate that the phytoplankton can contain per unit chlorophyll. The default value is 1 mmol (mg Chl)$^{-1}$. Nitrate assimilation decreases as this maximum quota is reached, and is zero at the maximum quota.

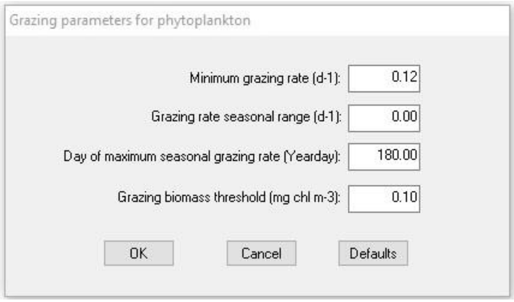
Nutrient concentration for half maximum uptake (mmol m^{-3}): the ambient concentration of dissolved inorganic nitrogen at which a nitrate-starved phytoplankton achieves half of the maximum nitrate uptake rate. The default value is 0.3 mmol m^{-3}. The value sets the steepness of the initial slope of the Michaelis-Menton uptake curve.

Subsistence cell nutrient quota (mmol N (mg Chl)$^{-1}$): the internal nitrate concentration, normalised by biomass, required before there can be phytoplankton growth. It is used in the model to modify the rate of photosynthesis. If the cell nitrate quota drops below the subsistence quota, biomass begins to be lost. The default value is 0.2 mmol (mg Chl)$^{-1}$. It should be greater than zero and less than the maximum cell nutrient quota.

Swimming speed (m d^{-1}): vertical swimming speed for the phytoplankton. The model only applies this speed during daylight, with swimming speed set to zero when it is dark. Positive speed is upward. Typical values might range between 1 and 10 m d^{-1}. Note that in the Eulerian framework of this type of model the application of a swimming (or sinking) speed is to the whole phytoplankton population. This framework is not well suited to swimming strategies that might depend on resource needs of phytoplankton cells; a Lagrangian modelling approach is then far preferable (e.g. Ross & Sharples, *Journal of Marine Systems*, **70**, 248-262, 2008).

Sinking speed (m d^{-1}): vertical sinking speed for the phytoplankton. The model applies this speed all the time. Set the speed to be negative for sinking.

3.7 ***Phytoplankton – Grazing:*** *controlling the loss of phytoplankton.*
Grazing of the phytoplankton is forced as a fraction of phytoplankton biomass removed each time step. It can be given a simple seasonal sinusoidal variability. The model default is a fixed value applied all year.



Minimum grazing rate (d^{-1}): the lowest grazing impact of the year. If a zero grazing rate range is set (see below), then this minimum grazing rate is the fixed grazing rate applied all year.

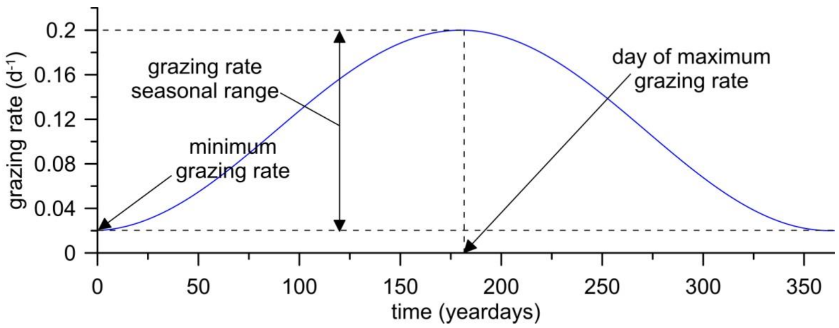
Grazing rate seasonal range (d^{-1}): the highest grazing rate of the year. This controls the seasonal variability of grazing applied through the year. Set it to zero (the default) for a fixed grazing rate (controlled by the minimum grazing rate, above).

Year day on which maximum grazing rate is reached: the day of the year (year day) on which the maximum grazing impact is reached. This parameter thus controls the phase of any seasonal variation in grazing impact.

The model calculates a grazing rate, g (d^{-1}), for each day of the year, t, from:

$$g(t) = g_{min} + \frac{g_{range}}{2}\left[1 + \cos\left(\omega_a (t - t_{max})\right)\right]$$

With g_{min} the minimum grazing rate, g_{range} the grazing rate seasonal range, ω_a (d^{-1}) the annual frequency and t_{max} the year day of maximum grazing. The following plot illustrates how these parameters control the seasonality of grazing:



Biomass threshold for grazing (mg Chl m^{-3}): threshold of chlorophyll concentration below which grazing is not applied. This allows simulation of grazers not feeding in low-biomass regions. It can be an important parameter in allowing phytoplankton to over-winter without needing to include some seed stock.

3.8 ***Oxygen****: fluxes and stoichiometry.*

This version of the S2P2 model includes dissolved oxygen as a state variable. Oxygen in the water column is influenced by the following processes:

(i) Air-sea flux of oxygen between the sea surface and atmosphere. The direction of the flux depends on the saturation state of dissolved oxygen in the surface grid cell. If saturation > 100%, then oxygen is released to the atmosphere; if saturation is < 100% then the surface grid cell absorbs oxygen from the atmosphere. The saturation state is a strong function of temperature (warmer water can hold less dissolved gas) and a weak function of salinity (which is constant at 35.0 in the model). The flux of oxygen is dependent on the difference between the oxygen saturation state and a saturation of 100%, and on the wind speed.

(ii) Phytoplankton photosynthesis, or carbon fixation, in a model grid cell adds oxygen to the grid cell. The amount of oxygen supplied to the water is set by a fixed oxygen:carbon stoichiometry.

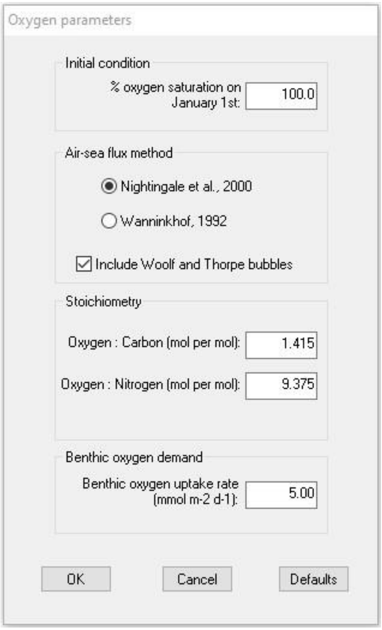
(iii) Phytoplankton respiration in a grid cell removes oxygen from that grid cell. Respiration is calculated in terms of respired carbon, and the oxygen consumed is set by the fixed oxygen:carbon stoichiometry.

(iv) Remineralisation of organic matter in a grid cell removes dissolved oxygen from the water in the grid cell. The model splits the organic detritus into two pools: slow-sinking and fast-sinking (or, small organic particles and big organic particles). Each of these pools is supplied with organic carbon and nitrogen from the grazing of phytoplankton. The remineralisation effect on dissolved oxygen is set by the oxygen:carbon and oxygen:nitrogen stoichiometry. The rates of remineralisation (i.e., the rates of oxygen consumption by remineralisation) can be different between the slow- and fast-sinking pools and also for carbon and nitrogen.

(v) The model does not include a benthic component, but we need to account for a benthic demand for oxygen as a part of the overall budget for water column dissolved oxygen. Benthic oxygen demand is included, which removes oxygen from the bottom grid cell.

(vi) Each of the processes above alters the dissolved oxygen concentrations in each of the grid cells in the modelled vertical profile. Once that has been done, the model then redistributes dissolved oxygen via vertical turbulent mixing.

The **Oxygen** and **Detritus** menus control key parameters in the biogeochemistry of dissolved oxygen production and consumption.



In the **Oxygen** menu:

Initial % oxygen saturation on January 1st: This sets the initial oxygen concentration vertical profile by calculating the oxygen concentration based on the initial saturation state. For the default value on January 1st (northern hemisphere winter) we expect the water column to be well-mixed, and exchange with the atmosphere will quickly drive the shelf water column dissolved oxygen close to 100% saturation.

Air-sea flux method: there are 2 commonly-used parameterisations of air-sea gas flux. You can choose one of:

1. Nightingale et al., *Global Biogeochemical Cycles*, 14(1), 373-387, 2000.
2. Wanninkhof, *Journal of Geophysical Research*, 97(C5), 7373-7382, 1992.

There is also the option to include the effects of enhanced air-sea flux associated with bubbles, following Woolf & Thorpe, *Journal of Marine Research*, 49, 435-466, 1991.

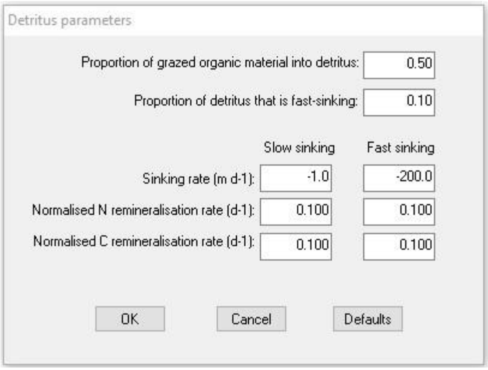
Within each grid cell in the modelled vertical profile, oxygen can be produced by photosynthesis (carbon fixation) or removed by respiration and by remineralisation or organic (cellular) nitrogen and carbon. How much oxygen is produced or removed is controlled by the stoichiometry of oxygen:carbon and oxygen:nitrogen.

Oxygen:Carbon (mol per mol): this controls the oxygen production by phytoplankton carbon fixation and the oxygen removal caused by respiration and by remineralisation of detrital organic carbon.

Oxygen:Nitrogen (mol per mol): this controls the oxygen removal caused by remineralisation of organic nitrogen. The organic nitrogen is the cellular nitrogen held by the phytoplankton. In a model grid cell, remineralisation of organic nitrogen results in inorganic nitrogen being returned to the dissolved inorganic nitrogen in the grid cell.

Benthic oxygen uptake (mmol m^{-2} day^{-1}): this is the total oxygen uptake rate by the benthos. This varies depending on sediment type (muddy sediments tend to host benthic communities with higher oxygen demand). The default value of 5 mmol m^{-2} day^{-1} is taken from measurements over a sandy seabed in the Celtic Sea (see: Hicks et al., *Biogeochemistry*, 135, 35-47, 2017).

*3.9 **Detritus**: controlling the fate of organic matter.*



Grazed organic phytoplankton carbon and nitrogen can be put into detrital organic carbon and nitrogen pools, which are then remineralised. The remineralisation of the organic detritus consumes oxygen, and so affects the dissolved oxygen in the water column. There are two pools of organic carbon and nitrogen: one a fast-sinking component (e.g. large phytoplankton cells or faecal pellets from zooplankton) and one a slow-sinking component (e.g. small phytoplankton or other organic particles, dissolved organic material). Each pool has its own sinking speed and separate remineralisation rates for organic carbon and nitrogen. As the pools have their own remineralisation rates, you could also view them as representing refractory and labile organic matter.

Proportion of grazed organic material into detritus: not all of the grazed organic material becomes detrital. Some of it is passed further up the food chain, some of it could be highly refractory (i.e. not available for remineralisation on the timescale of a model run), some of it could be buried in sediments. The model default is 50% of grazed material being put into the detrital pools. This parameter exerts a key control on bottom water dissolved oxygen concentrations when the water column is stratified.

Proportion of detritus that is fast sinking: this controls how the detrital material is split between the fast- and slow-sinking pools.

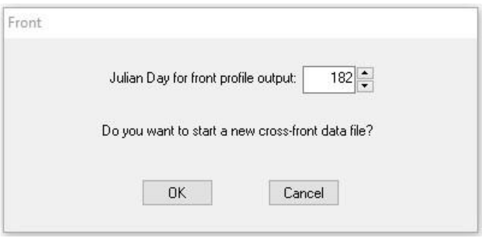
Slow-sinking and fast-sinking organic carbon and nitrogen pools each have:

Detrital sinking rate (m day^{-1}): sinking speed of the organic carbon and nitrogen. This needs to be negative to sink.

Normalised N remineralisation rate (day^{-1}): rate of organic nitrogen remineralisation. Remineralisation of detrital organic nitrogen in a model grid cell will reduce the dissolved oxygen in the grid cell (based on the stoichiometry in the oxygen menu). Remineralised organic nitrogen also results in a corresponding increase in the dissolved inorganic nitrogen in the grid cell. Thus, remineralisation of organic nitrogen replenishes nutrient that is immediately available for phytoplankton uptake.

Normalised C remineralisation rate (day^{-1}): rate of organic carbon remineralisation. Remineralisation of detrital organic carbon in a model grid cell will reduce the dissolved oxygen in the grid cell (based on the stoichiometry in the oxygen menu).

*3.10 **Cross front**: synthesising a 2-D section.*



The model can be used to synthesise a 2-D section through a shelf sea front, by running it several times with different tidal and/or depth parameters. The same approach has been used in:

> Sharples, J. and J.H.Simpson. 1996. The influence of the springs-neaps cycle on the position of shelf sea fronts. In: *Buoyancy Effects on Coastal Dynamics*, D.G.Aubrey & C.T.Friedrichs (Eds). Coastal and Estuarine Studies Volume 53, AGU, 71-82.
>
> Sharples, J. 2008. Potential impacts of the spring-neap tidal cycle on shelf sea primary production. *Journal of Plankton Research*, **30(2)**, 183-197.

The success of the approach is because of the dominance of the vertical heating-mixing competition in setting the vertical structure of the NW European shelf seas. It may not be appropriate everywhere.

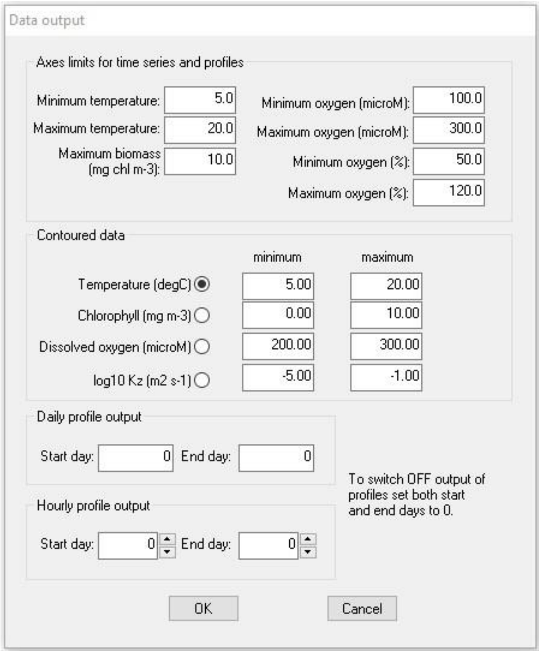
At the day specified in the **front** dialog the model outputs vertical profiles at noon into an ASCII data file front_data.dat with the following columns:

SH: $\log_{10}(h/u^3)$, the Simpson-Hunter stratification parameter; u^3 here is the long-term average of the depth-mean current speed cubed.
depth: depth below the sea surface (metres). These depths mark the centres of the model grid cells, where the scalars and velocity are located.
temp: temperature (^oC) at depth, noon value.
chl: noon concentration of chlorophyll (mg m^{-3}) at depth.
chlC: noon concentration of organic carbon (mg m^{-3}) at depth.
cellN: noon concentration of cellular nitrogen (mmol m^{-3}) at depth.
uptake: amount of dissolved inorganic nitrogen (mmol m^{-3}) taken up at depth in the previous 24 hours.
netPP: net primary production (mg C m^{-3}), or net carbon fixed, at depth over the previous 24 hours.
grossPP: gross primary production (mg C m^{-3}), or gross carbon fixed, at depth over the previous 24 hours.
DIN: noon concentration of dissolved inorganic nitrogen (mmol m^{-3}) in the water at depth.
O2: noon concentration of dissolved oxygen (microM) in the water at depth.
fastN: noon concentration of fast-sinking detrital organic nitrogen (mmol m^{-3}) in the water at depth.
slowN: noon concentration of slow-sinking detrital organic nitrogen (mmol m^{-3}) in the water at depth.
fastC: noon concentration of fast-sinking detrital organic carbon (mmol m^{-3}) in the water at depth.
slowC: noon concentration of slow-sinking detrital organic carbon (mmol m^{-3}) in the water at depth.
hKz: depth below the sea surface (metres). These depths mark the boundaries between grid cells, where Kz (vertical eddy diffusivity) is located.
logKz: log10 of the vertical eddy diffusivity ($m^2\ s^{-1}$) at depth hKz. The output value is a noon to noon average of 24 hourly values.

As long as "Cross front" is not chosen again, or the model is not closed and re-started, the profile data at the specified time is appended to the end of the front data file for each new run. If "Cross front" is selected, or the model is shut down and then re-started, then the front data file will be over-written. So, remember to re-name the front data file if you wish to keep it.

3.11 ***Save screen***
The model graphical output can be saved as a bitmap image file, either at the end of a model run or after pressing <escape> partway through a run. Select **Save screen** from the main menu and provide a filename for the bitmap as prompted.

*3.12 **Data output**: controlling graphical and data file outputs.*



<u>Screen Graphics.</u>
Changes can be made to some of the graphical output used in the screen plots of model data.

In the *Axes limits for time series and profiles* section:

Minimum and maximum temperature, maximum biomass, and the minimum and maximum concentrations of dissolved oxygen control the y-axis limits in the annual time series plot of surface and near-bed temperature, surface chlorophyll and near-bed dissolved oxygen.

The minimum and maximum oxygen saturation (%) controls the x-axis limits for the vertical profile plot of oxygen saturation.

In the *Contoured data section*:
You can select 1 out of 4 possible variables to plot as colour-shaded contours through the annual time series. In each case you can also specify the range over which the contours will be plotted.

<u>Output to data files.</u>
The model outputs several datafiles during operation. Each file has a default filename which is over-written on each model run. See below for descriptions of the data sent to the various output files.

Daily and hourly summary data:
This data output is always switched on, with data going to the files "daily_summary.dat" and "hourly summary.dat". Daily summary data is output at each model noon. Unless stated otherwise below, output data are instantaneous values at noon for the daily data or at each hour for the hourly data. These summary data files are ASCII text files with the following columns:

JD : Julian Day (JD=1 on January 1st, 365 or 366 (leap year) on December 31st).
hr: output in the hourly summary file only, hour of the day from 0 (midnight) to 23.
time: time (decimal year days).
SH: log10(h/u^3), the Simpson-Hunter stratification parameter; u^3 here is the long-term average of the depth-averaged current speed cubed.
Ts: sea surface temperature (°C)
Tb: near-bed sea temperature (°C)
Ts-Tb: surface-bottom temperature difference (°C)
PHI: potential energy anomaly ($J\ m^{-3}$)

spd: daily-mean, depth-averaged current speed (m s^{-1}). This is a daily mean in the daily summary output, or an instantaneous value in the hourly data.
stress:surface wind stress (N m^{-2}). This is a daily mean in the daily summary output, or an instantaneous value in the hourly data.
Qs: surface solar radiation (W m^{-2}). This is a daily mean in the daily summary output, or an instantaneous value in the hourly data.
Qflux: net surface heat flux, positive is heat into the sea surface (W m^{-2}). This is a daily mean in the daily summary output, or an instantaneous value in the hourly data.
CHLs: surface chlorophyll concentration (mg m^{-3})
Cs: surface phytoplankton carbon concentration (mg m^{-3})
CHLt: depth-integrated chlorophyll (mg m^{-2})
Ct: depth-integrated phytoplankton carbon (mg m^{-2})
DINs: surface concentration of dissolved inorganic nitrogen (mmol m^{-3})
netp: net daily water column primary production (g C m^{-2} d^{-1} or g C m^{-2} hr^{-1}). This is a daily mean in the daily summary output, or an hourly mean in the hourly data. Note that the net primary production is calculated at each model time step as the gross primary production minus respiration.
grossp: gross daily water column primary production (g C m^{-2} d^{-1} or g C m^{-2} hr^{-1}). This is a daily mean in the daily summary output, or an hourly mean in the hourly data.
O2flux: air-sea flux of oxygen (mmol m^{-2} day^{-1} or mmol m^{-2} hr^{-1}). This is a daily mean in the daily summary output, or an instantaneous value in the hourly data. Negative flux is a loss of oxygen from the sea surface to the atmosphere.
O2surf: surface grid cell dissolved oxygen concentration (microM).
O2%surf: surface grid cell dissolved oxygen % saturation.
O2bed: bottom grid cell dissolved oxygen concentration (microM).
O2%bed: bottom grid cell dissolved oxygen % saturation.
fastCsur: surface grid cell fast-sinking detrital carbon (mmol m^{-3}).
fastNsur: surface grid cell fast-sinking detrital nitrogen (mmol m^{-3}).
slowCsur: surface grid cell slow-sinking detrital carbon (mmol m^{-3}).
slowNsur: surface grid cell slow-sinking detrital nitrogen (mmol m^{-3}).
fastCbed: bottom grid cell fast-sinking detrital carbon (mmol m^{-3}).
fastNbed: bottom grid cell fast-sinking detrital nitrogen (mmol m^{-3}).
slowCbed: bottom grid cell slow-sinking detrital carbon (mmol m^{-3}).
slowNbed: bottom grid cell slow-sinking detrital nitrogen (mmol m^{-3}).

Monthly summary data:
This data output is always switched on, with data going to the default file "monthly_summary.dat". Note that the months are set up for the case of the northern hemisphere (model run starts on January 1st), so the timing of the months will not be correct for the southern hemisphere (in that case either treat this output as a reasonable estimate or use the information in the daily summary data file to calculate a better result).

Data is output at the end of each month, as an ASCII text file with the following columns:

month: January = 1, December = 12. Days in each month are based on a non-leap year. This is only applicable to the northern hemisphere.
SH: log10(h/u3), the Simpson-Hunter stratification parameter; u3 here is the long-term average of the depth-averaged cubed current speed.
Ts: monthly mean sea surface temperature (^oC).
Tb: monthly mean near-bed water temperature (^oC).
delta-T: monthly mean surface-bottom temperature difference (^oC).
Wstress: monthly mean wind stress (N m^{-2}).
Chlt: monthly mean water column integrated chlorophyll (mg Chl m^{-2}).
Ct: monthly mean water column integrated organic carbon (g C m^{-2}).
Cgross: total gross carbon fixed in the month (g C m^{-2}).
Cnet: total net carbon fixed in the month (g C m^{-2}).
accumC: net carbon fixed since January 1st (g C m^{-2}).

Daily and hourly profiles:
Output to data files of vertical profiles is set within the *Daily profile output* and *Hourly profile output* sections. Profiles are only saved if End day > Start day. If End day = Start day = 0 no profile data files

are opened. Instantaneous vertical profiles of physical and biogeochemical data are output at noon (daily profiles) or at each hour (hourly profiles), unless otherwise stated below. Data are written into ASCII files with the following columns:

Physics profiles.
Filenames "phys_profiles_day.dat" and "phys_profiles_hour.dat".

time: decimal days with time=0.0 at 0000 hrs January 1st.
hu3: $\log_{10}$ of the Simpson-Hunter parameter SH=h/u^3, with h the water depth and u^3 the long-term depth-average current speed cubed.
depth: depth below the sea surface (metres). These depths mark the centres of the model grid cells, where the scalars and velocity are located.
temp: temperature (^{o}C) at depth.
sigmat: density-1000 kg m^{-3} at depth.
u: east-west current velocity component (m s^{-1}) at depth, instantaneous or averaged over 24 hours (noon to noon). Positive values to the east.
v: north-south current velocity component (m s^{-1}) at depth, instantaneous or averaged over 24 hours (noon to noon). Positive values to the north.
z_turb: depth below the surface (metres). These depths mark the boundaries between grid cells, where the turbulence parameters are located.
Ri: gradient Richardson number at depth z_turb. Ri is constrained to lie between -1.0 and 10.0; i.e. if Ri > 10.0, Ri is output at 10.0. The output value is either an hourly average or a noon to noon average.
logKz: $\log_{10}$ of the vertical eddy diffusivity (m^2 s^{-1}) at depth z_turb. The output value is either an hourly average or a noon to noon average.
logdiss: $\log_{10}$ of the turbulent dissipation (m^2 s^{-3}) at depth z_turb. The output value is either an hourly average or a noon to noon average.
logtke: $\log_{10}$ of the turbulent kinetic energy (m^2 s^{-2}) at depth z_turb. The output value is either an hourly average or a noon to noon average.

Note that the turbulence variables are specified on the boundaries between grid cells. This means that the surface values are set at a depth of z_turb=0 metres (i.e. the top face of the top grid cell). The values here drop very quickly compared to those at the base of the top grid cell, largely because of the way the turbulent length scale decreases towards the boundary. However, the turbulence at z_turb=0 metres does not have any effect on the structure of the scalars in the water column. Mixing of quantities between the top grid cell and the grid cell immediately below it is controlled by the turbulence at the base of the top grid cell.

Biological profiles.
Filenames "bio_profiles_day.dat" and "bio_profiles_hour.dat".

time: decimal days with time=0.0 at 0000 hrs January 1st.
hu3: $\log_{10}$ of the Simpson-Hunter parameter SH=h/u^3, with h the water depth and u^3 the long-term depth-average current speed cubed.
depth: depth below the sea surface (metres). These depths mark the centres of the model grid cells, where the scalars and velocity are located.
PAR: mean PAR (W m^{-2}) received within the model grid cell centred at depth. Instantaneous value in hourly profiles, or noon to noon average in daily profiles.
chl: concentration of chlorophyll (mg m^{-3}) at depth.
cellC: concentration of phytoplankton carbon (mg m^{-3}) at depth.
cellN: concentration of cellular nitrogen (mmol m^{-3}) at depth.
netPP: net primary production (mg C m^{-3} hr^{-1} or mg C m^{-3} day^{-1}), or net carbon fixed, at depth averaged over 1 hour or over the previous 24 hours. Note that the net primary production is calculated at each model time step as the gross primary production minus respiration.
grossPP: gross primary production (mg C m^{-3} hr^{-1} or mg C m^{-3} day^{-1}), or gross carbon fixed, at depth averaged over 1 hour or over the previous 24 hours.
uptake: amount of dissolved inorganic nitrogen (mmol m^{-3} hr^{-1} or mmol m^{-3} day^{-1}) taken up at depth averaged over 1 hour or over the previous 24 hours.
DIN: concentration of dissolved inorganic nitrogen (mmol m^{-3}) in the water at depth.

Oxygen profiles.
Filenames "oxygen_profiles_day.dat" and "oxygen_profiles_hour.dat".

time: decimal days with time=0.0 at 0000 hrs January 1st.
hu3: $\log_{10}$ of the Simpson-Hunter parameter SH=h/u^3, with h the water depth and u^3 the long-term depth-average current speed cubed.
depth: depth below the sea surface (metres). These depths mark the centres of the model grid cells, where the scalars and velocity are located.
Ox: dissolved oxygen concentration (microM) at depth.
Ox%: dissolved oxygen saturation (%) at depth.
Photo: contribution of photosynthesis to changes in dissolved oxygen at depth (microM hr^{-1} or microM day^{-1}).
Resp: contribution of respiration to changes in dissolved oxygen at depth (microM hr^{-1} or microM day^{-1}).
Ndetritus: contribution of emineralisation of detrital nitrogen to changes in dissolved oxygen at depth (microM hr^{-1} or microM day^{-1}).
Cdetritus: contribution of remineralisation of detrital carbon to changes in dissolved oxygen at depth (microM hr^{-1} or microM day^{-1}).
diapyc: contribution of turbulent mixing of dissolved oxygen to changes in dissolved oxygen at depth (microM hr^{-1} or microM day^{-1}). Note this is not the diapycnal oxygen flux: it is the net change in concentration caused by diapycnal fluxes.

Detritus profiles.
Filenames "detritus_profiles_day.dat" and "detritus_profiles_hour.dat".

time: decimal days with time=0.0 at 0000 hrs January 1st.
hu3: $\log_{10}$ of the Simpson-Hunter parameter SH=h/u^3, with h the water depth and u^3 the long-term depth-average current speed cubed.
depth: depth below the sea surface (metres). These depths mark the centres of the model grid cells, where the scalars and velocity are located.
FastN concentration of fast-sinking detrital nitrogen (mmol m^{-3}).
SlowN concentration of slow-sinking detrital nitrogen (mmol m^{-3}).
FastC concentration of fast-sinking detrital carbon (mmol m^{-3}).
SlowC concentration of slow-sinking detrital carbon (mmol m^{-3}).
Nremin remineralisation rate of detrital nitrogen (mmol m^{-3} hr^{-1} or mmol m^{-3} day^{-1}). Instantaneous hourly rate or daily-averaged rate.
Cremin remineralisation rate of detrital carbon (mmol m^{-3} hr^{-1} or mmol m^{-3} day^{-1}). Instantaneous hourly rate or daily-averaged rate.

3.13 ***Help.***
The **Help** option in the main menu provides you with almost all of the information in this guide, via the **Instructions** option. Note also the **About** option, which includes the model version number and an all-important disclaimer.

4. Final Comments.
While I have shirked responsibility for any bugs or errors existing in the model in the disclaimer, I am keen that new errors are found and fixed. If you find an error, or if you have any suggestions for improvements or additions to the model (e.g. to the types of data output for instance), then I will be happy to hear about them. I will endeavour to fix any errors found. I will make other alterations/ additions depending on demand and time constraints. Modified version of the model will be posted on my website, along with notes on the changes that have been made.

Jonathan Sharples
http://pcwww.liv.ac.uk/~jons/index.htm
jons@liverpool.ac.uk
22nd March 2023
