Supplement of

Optimality-based non-Redfield plankton–ecosystem model (OPEM v1.1) in UVic-ESCM 2.9 – Part 2: Sensitivity analysis and model calibration

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Figure S1 shows the deep-water oxygen distribution in a simulation with very low globally averaged oxygen concentration (111 mmol O$_2$ m$^{-3}$). Figures S2 to S7 show how neglecting variation, correlation, and both variation- and correlation-components affect the global mean tracer concentrations and flux estimates of our simulations.

The second part of this supplemental material are the instructions to reproduce the model results described in the main article.

**Figure S1.** Oxygen concentration in the deep water (1240 to 5490 m) of a simulation with very low globally averaged oxygen (111 mmol O$_2$ m$^{-3}$). Purple color (< 5 mmol O$_2$ m$^{-3}$) indicates the distributions of oxygen deficient zones (ODZs). This simulation is the same one as the low nitrate OPEM simulation shown in Figure 6 of the main article.
Figure S2. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. N\textsubscript{2} fixation in the OPEM and OPEM-H configurations. Red and blue symbols and lines are for OPEM (triangles) and OPEM-H (circles), respectively. Solid and open symbols represent minimum-cost and trade-off simulations, respectively. Vertical solid and dashed lines represent means and 95% confidence intervals of best solutions of 1000 randomly selected subsets of 100 ensemble members. Red parabolas fit the lowest costs at different rates or tracer concentrations. Note that we only show one side of the red parabolas here because N\textsubscript{2} fixation rates with the minimum cost values are close to zero.

Figure S3. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. NO\textsubscript{3}\textsuperscript{−}, symbols and colors are defined identically to Figure S2.
Figure S4. Cost values (A), and partial costs omitting the variance-components (B), omitting the correlation-components (C), and omitting both correlation- and variance-components (D) vs. O$_2$, symbols and colors are defined identically to Figure S2.

Figure S5. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. DIC, symbols and colors are defined identically to Figure S2.
Figure S6. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. NPP, symbols and colors are defined identically to Figure S2.

Figure S7. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. NCP, symbols and colors are defined identically to Figure S2.
Manual
UVic-OPEM Set-Up, Calibration, and Reference Simulations

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1 Setting up UVic-OPEM

1.1 Prerequisites
In order to compile and run UVic-OPEM, first the programs bash, perl, and a Fortran-90 compiler must be installed. Then the netcdf library and its Fortran interface must be compiled with the same Fortran compiler to be used for UVic-OPEM. When installing pre-compiled netcdf libraries, make sure it was compiled with the same Fortran compiler as used in your system.

1.2 Obtaining and compiling the code

1. You can obtain the base UVic code from [http://www.climate.uvic.ca/model/](http://www.climate.uvic.ca/model/) and unpack it inside the updates folder.

2. Change to the updates folder.

3. Download the OPEM v1.1 code from [https://dx.doi.org/10.3289/SW_1_2020](https://dx.doi.org/10.3289/SW_1_2020) and unpack it inside the updates folder.

4. Create another directory, <run> in the following, preferably outside of <base>, change to there, and create two sub-folders, <run>/orig and <run>/OPEM.

5. Copy mk.in_orig to <run>/orig/mk.in and mk.in_OPEM to <run>/OPEM/mk.in.

6. Open <run>/orig/mk.in with a text editor and replace <base> on line 5 with the actual path.

7. In order to obtain the Original UVic executable, change to <run>/orig and issue the command <base>/mk -e to compile the code. This should generate the executable <run>/orig/UVic_ESCM (specified towards the end of <run>/orig/mk.in as Executable_File). If the compilation failed, examine the file <run>/orig/mk.log for error messages.

8. For the OPEM executable (this is the same for both the OPEM and OPEM-H configurations), repeat the previous step for <run>/OPEM.

2 Reference (trade-off) simulations

For the reference (trade-off) simulations, create three new folders, e.g., <run>/ref_orig, <run>/ref_OPEM and <run>/ref_OPEM-H, and copy the executables and data folders there (they are the same for OPEM and OPEM-H). Copy <base>/updates/opem/restarts/restart_* .nc. The place the control.in_orig, control.in_OPEM and control.in_OPEM-H there as well. Assuming you downloaded the control.in_* files to <run>:
The you can obtain the 1-year reference simulation for the original UVic with

```
cd <run>
mkdir ref_orig
mkdir ref_OPEM
mkdir ref_OPEM-H
cp -pr <run>/orig/{UVic_ESCM,data} ref_orig/
cp -pr <run>/OPEM/{UVic_ESCM,data} ref_OPEM/
cp -pr <run>/OPEM/{UVic_ESCM,data} ref_OPEM-H/
cp -pf <base>/updates/opem/restarts/restart_orig.nc <run>/ref_orig/data/restart.nc
cp -pf <base>/updates/opem/restarts/restart_OPEM.nc <run>/ref_OPEM/data/restart.nc
cp -pf <base>/updates/opem/restarts/restart_OPEM-H.nc <run>/ref_OPEM-H/data/restart.nc
cp -p control.in_orig ref_OPEM/control.in
cp -p control.in_OPEM ref_OPEM-H/control.in
```

and analogously for OPEM and OPEM-H. Note that these simulations assume that the year has 360 days. Thus, the time integrals must be multiplied with 365/360 to obtain annual rates.

### 3 Calibration simulations for OPEM and OPEM-H

#### 3.1 Compile UVic_ESCM

The calibration simulations can be set up with the files in `<base>/updates/opem/calibration`. For these simulations we used 365-day years, so the UVic_OPEM must be recompiled with a different `mk.in`:

```
cd <run>
mkdir calib
cp -p <base>/updates/opem/{mk.in,calibration/*} calib/
```

Now, again, edit `calib/mk.in`, replacing `<base>` with its actual path, and compile:

```
cd calib
;base>/mk -e
```

#### 3.2 Creating parameter files

Inside the calibration folder (`<run>/calib`) create two new folders, OPEM and OPEM-H and create the 400 `control_*` files in each of them:

```
mkdir OPEM
mkdir OPEM-H
cd OPEM
"./write_control ./control.in.OPEM
cd ../OPEM-H
"./write_control ../control.in.OPEM-H
```

The script `write_control` substitutes the 400 parameter combinations in the file `parameter.txt` in the `control.in` templates. The `control_*` files are set up for 100,000-year simulations in steps of 1000 years. In order to do these simulations, set up 400 folders, copy the `<run>/calib/UVic_ESCM` and `<run>/calib/data` there, and distribute the `control_*` files to `<run>/calib/{OPEM,OPEM-H}/`.