Supplemental Material: Optimality-Based Non-Redfield Ecosystem Model in the UVic-ESCM. Part II: Sensitivity Analysis and Model Calibration

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The supplemental figures (Figure S1 to S6) show how neglecting variation, correlation, and both variation- and correlation-components affect the global mean tracer concentrations and flux estimates of our simulations. Second part of this supplemental material are the instructions to reproduce the model results described in this article.
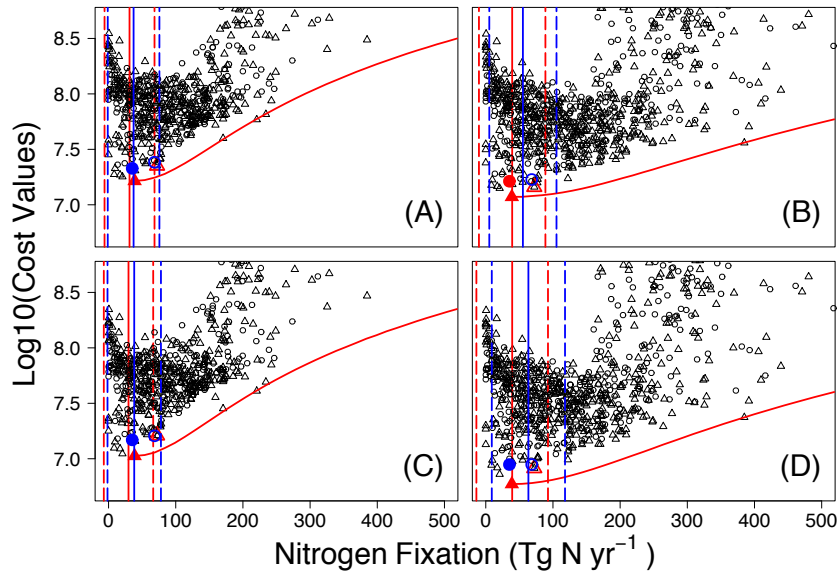
Figure S1. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. N_2 fixation in the OPEM and OPEM-H configurations. Red and blue symbols and lines are for OPEM (triangles) and OPEM-H (circles), respectively. Solid and open symbols represent minmum-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_2 fixation rates with the minimun cost values are close to zero.
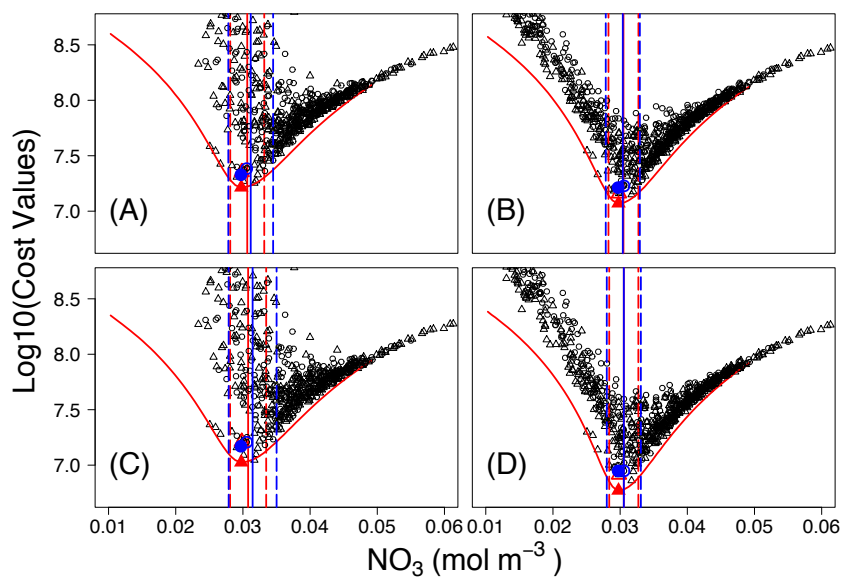
Figure S2. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. NO_3^-, symbols and colors are defined identically to Figure S1.
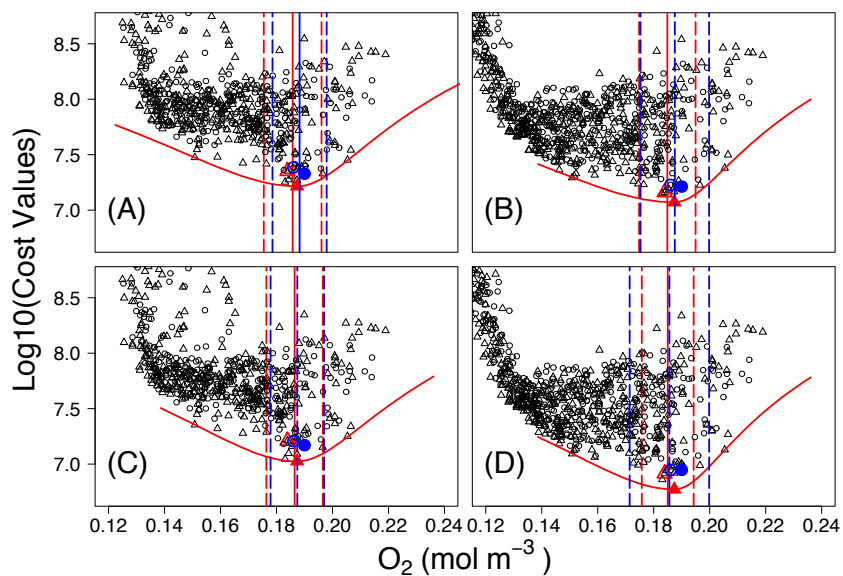
Figure S3. Cost values (A), and partial costs omitting the variance-components (B), omitting the correlation-components (C), and omitting both correlation- and variance-components (D) vs. O_2, symbols and colors are defined identically to Figure S1.
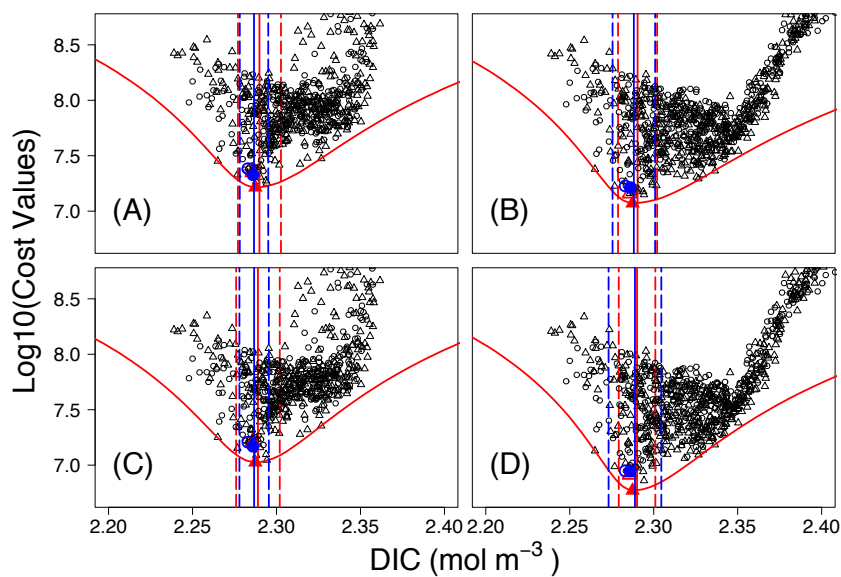
Figure S4. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. DIC, symbols and colors are defined identically to Figure S1.
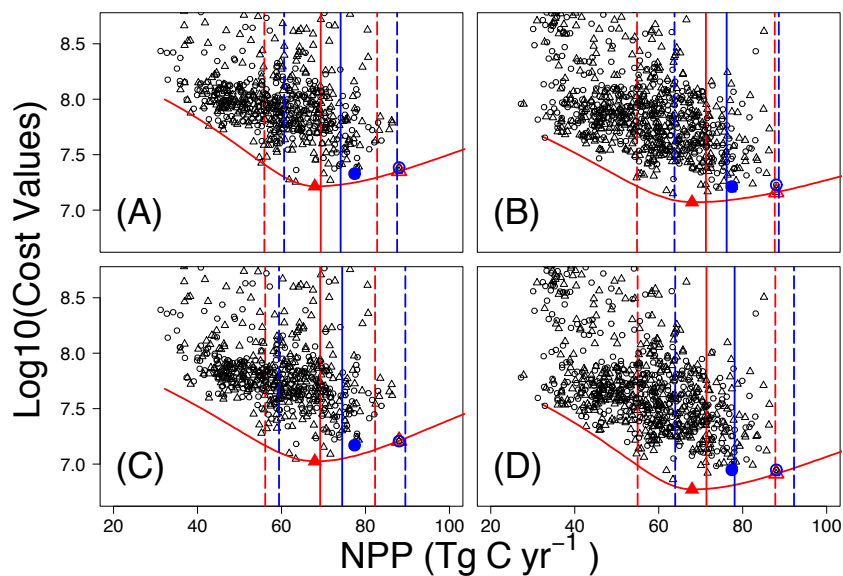
Figure S5. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. NPP, symbols and colors are defined identically to Figure S1.
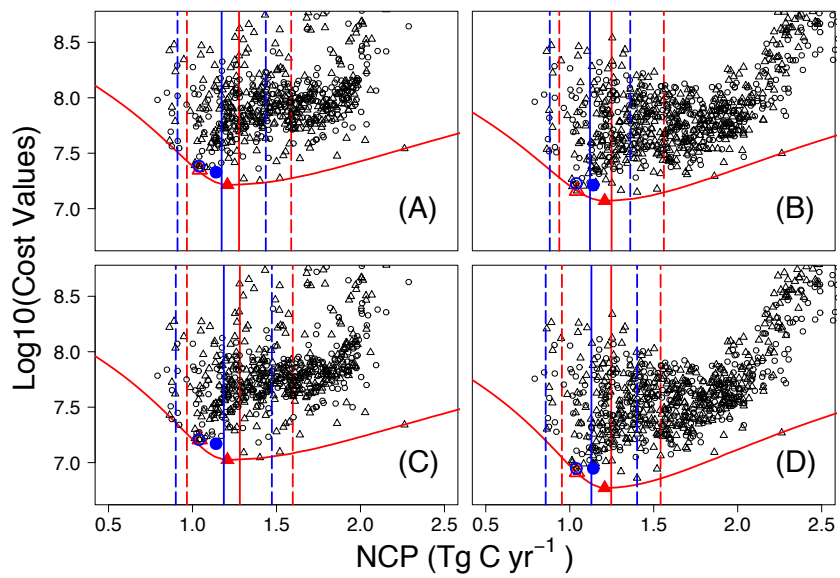
Figure S6. Cost values (A), and partial costs omitting variation-components (B), omitting correlation-components (C), and omitting correlation- and variation-components (D) vs. NCP, symbols and colors are defined identically to Figure S1.

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/. Switch to a directory selected for your UVic-OPEM installation, untar the base UVic code there, and change to the directory thus created. In the following, this directory will be referred to as <base>.

2. Change to the updates folder.

3. Download the OPEM v1.0 code from http://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. 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. 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 dowloaded the control.in_* files to <run>:

```
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_orig/control.in
cp -p control.in_OPEM ref_OPEM/control.in
cp -p control.in_OPEM-H ref_OPEM-H/control.in
```

Then you can obtain the 1-year reference simulation for the original UVic with

```
cd <run>/ref_orig
UVic_ESCM > log
```

and analogously for OPEM and OPEM-H. Note that these simulations assume that the year has 360 days. Thus, the time integrals mus 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_*.in.in 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_*.in.in 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_*.in.in files to <run>/calib/{OPEM,OPEM-H}/*/control.in.