A simple box model for the geochemical cycling of iron in the ocean

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1 Overview

This project contains matlab code to model the distribution of dissolved iron, phosphate and of zero, one or two organic iron-binding ligands in the ocean. The ocean is discretized into 12 boxes, representing main water masses in the Atlantic and Indo-Pacific ocean. Boxes are assumed to be homogeneously mixed and the ocean circulation is prescribed as exchanges between these boxes.

The model has been used to explore feedbacks in the ocean iron cycle connected to organic iron complexation (manuscript in preparation). The full model description can be found there.

The code presented here does not only contain the core model, but several additional tools. It is grouped broadly into the the following four parts:

2 Code to integrate the model and to analyse ligand feedbacks:

Several different versions of the box model exist, differing in the number of modeled quantities in each box (`boxmodel_po4.m` for example solves only one quantity, namely the phosphate concentration, while `boxmodel_po4dopfe2lig_export.m` solves for five quantities, namely phosphate, dissolved organic phosphorus, iron, and two ligands), and in whether export production is calculated from nutrients (all models ending with `_export.m`), or prescribed.

Running the models results in two output files, which are both found in the subdirectory `results`: One ASCII-file containing the final steady state concentration of the models state variables in all 12 model boxes in a table (`equil*.dat`), and one binary matlab file that documents the parameter values used in that model run (`parameters*.mat`).

Each of these models first calls the routine `boxmodel_init_params.m` to initialize all model parameters, including the volume of the boxes, and the mass transports between them. The parameters are transferred in the form of a global structure variable.

Each of the models then uses a matlab-provided routine to integrate stiff ordinary equations to integrate the model into equilibrium, passing the name of the routine that contains the right hand side of the corresponding box model differential equations to this routine. These routines have names `boxmodel_dgl_*.m`.

In the equations with prognostic ligands, one important step is to calculate the 'free', i.e. not organically complexed iron concentration. In the case of one or two organic ligands this boils down to finding the roots of either a quadratic or cubic polynomial. I also experimented with one version where a third weaker ligand was assumed to be present in constant concentration, as a representation maybe of humic substances. In that case, I created an extra function for the calculation of free iron, `func_feprime_tree_ligands.m`.

Feedbacks between biological production and organic iron complexation are calculated by running one of the model variants with prognostic (i.e. variable) ligands into equilbrium, then saving the resulting steady-state ligand concentration, and then running the model again (under some changed external condition, such as dust iron input), but this time with ligands held fixed at the previous steady state. This is done by the routines `feedback_loop_po4dopfelig.m` and `feedback_loop_po4dopfe2lig.m`. These routines also need additional differential equation routines which solve for phosphate, DOP and iron, but take the ligand concentration as spatially variable from the previous run with variable ligands. They are called `boxmodel_dgl_po4dopfe_ligfix_export.m` and `boxmodel_dgl_po4dopfe_2ligfix_export.m`.

The result from running the feedback analysis is saved in the directory `results` as a matlab binary file `feedback_*.mat`.

3 Routines to plot and analyse model output:

After running the models, or running the feedback analyses, the output can be plotted using the generated output in the `results` directory. The plotting routines also print out some basic analyses of the model output to the screen. Four different plots are provided:

`plot_po4_allmodels_bright.m` plots modeled phosphate concentrations in the twelve model boxes against the average phosphate concentration within the model boxes from the World Ocean Atlas 2009. `plot_po4_allmodels.m` is an older version with less nice colours.

`plot_dfe_allmodels_bright.m` plots modeled dissolved iron concentration against meadin and quantiles of observed dissolved iron from the second GEOTRACES intermediate data product.

`plot_ligands_allmodels_bright.m` plots the steady state ligand concentrations for all model boxes. Since the database for observed ligand concentrations is to small for creating reliable median values for the boxes, no observation data is plotted.

And finally, `plot_feedbacks_allmodels_bright.m` plots the variations of a number of important quantities (e.g. global average dissolved iron, and total global export production) as a function of external dust input, with and without the feedback.

All plotting routines are set up for plotting not only one model run or one feedback analysis, but comporing several model runs.If you want to plot just one output of a model run you will have to modify them slightly.

4 Code for setup of the model boxes and data sets:

The parts of the code described here are not necessary if you just intend to play around with model as it is now, but they may be helpful if you e.g. want to extend the model by adding more boxes, or to introduce new/additional data sets to compare model output with.

The first step for setting up the model is to calculate the volumes and, in the case of surface boxes, the surface area of the boxes, which is done in `calc_boxes_for_model.m`. The same routine also calculates the average phosphate concentration within the boxes from World Ocean Atlas 2009 data, and the total export production in each surface box from the estimate by Schlitzer et al. The routine uses a helper function `read_one_netcdf.m` to read the netcdf files for these data sets.

To do so, the routine requires several data sets that are not distributed here with the code, but that should be easily downloadable from the web. The required files are (names should be clickable links)

- World Ocean Atlas 2009 annual average distribution of potential temperature
- World Ocean Atlas 2009 annual average distribution of salinity
- World Ocean Atlas 2009 annual average distribution of phosphate
- World Ocean Atlas basin mask (n.b.: to avoid a confusing filename `data.nc` that file is renamed to `basinmask.nc`, and it is read as such in the routine).

In addition, the routine uses the seawater equation of state `swstate.m` from the WHOI seawater package, which can be downloaded here, to calculate potential density from temperature and salinity.

For modelling the iron cycle, external fluxes of iron into the ocean are required. In the present model, three sources of iron are taken into account, namely dust deposition, sediment iron release and hydrothermal input. The fluxes from these sources are calculated in `integrate_dust_for_boxmodel.m`, `calc_sediment_for_boxmodel.m`, and `calc_hydrothermal_for_boxmodel.m`. Again, these routines require files that are not distributed here with the model:

- dust deposition is calculated from the deposition field by Luo and Mahowald; I obtained that field by writing to Natalie Mahowald. It should be easy to use other dust deposition files instead, e.g. Albani et al.

- sediment iron fluxes are calculated from water depth, using the ETOTP 2 arc-minutes global topography.
- hydrothermal iron fluxes are calculated from hydrothermal helium fluxes, as described in Tagliabue 2010

Finally, the iron concentrations in the model are compared to values obtained from the GEOTRACES second intermediate data product bottle data, which can be downloaded from here. The routine to read the GEOTRACES data, sort it into the model boxes, and calculate quantiles for the individual boxes is `sort_fe_data_into_boxes.m`.

5 Routines to optimise parameters of the model: