DOCUMENTATION of BETR-Research 3.0

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1. Introduction

1.1. History of Berkeley-Trent (BETR) Models

BETR-Research 3.0 is the newest member of the Berkeley-Trent (BETR) family of spatially-explicit multimedia chemical fate and transport models. The list below presents BETR family of models in chronological order together with the main references for each model:

- BETR North America (MacLeod et al. 2001)
- European Variant Berkeley-Trent (Evn-BETR) (Prevedouros et al. 2004)
- BETR-World (Toose et al. 2004)
- BETR-Global (Macleod et al. 2005)
- BETR-Global 2.0 & BETR-Research (MacLeod et al. 2011)
- BETR-Research 3.0 (2016)

1.2. BETR-Research

The first version of BETR-Research was based on BETR-Global 2.0, which is a well-developed and tested global fate model implemented in Visual Basic for Applications (MacLeod et al., 2011). BETR-Research was developed by re-implementing BETR-Global 2.0 in the Python programming language. The purpose of this re-implementation was to create a more flexible modeling platform using BETR-Global's model structure and taking advantage of efficient numerical packages in Python.

Figure 1.1 presents the global grid of BETR-Global 2.0 and BETR-Research at 15°×15° resolution. At this resolution the global environment is divided into 288 model regions.

Figure 1.2 is a representation of the environmental compartments included in the model regions of BETR-Global 2.0 and BETR-Research. The multimedia environment is represented as a collection of seven compartments in interaction with each other. Obviously, not all the environmental regions contain all of the seven compartments. The compartment volumes and other environmental characteristics are described for all the model regions. These descriptions are provided to the model within specifically formatted input files in BETR-Research.

In recent years, the BETR-Research model source code has gone through several important modifications that lead to the new version: BETR-Research 3.0.

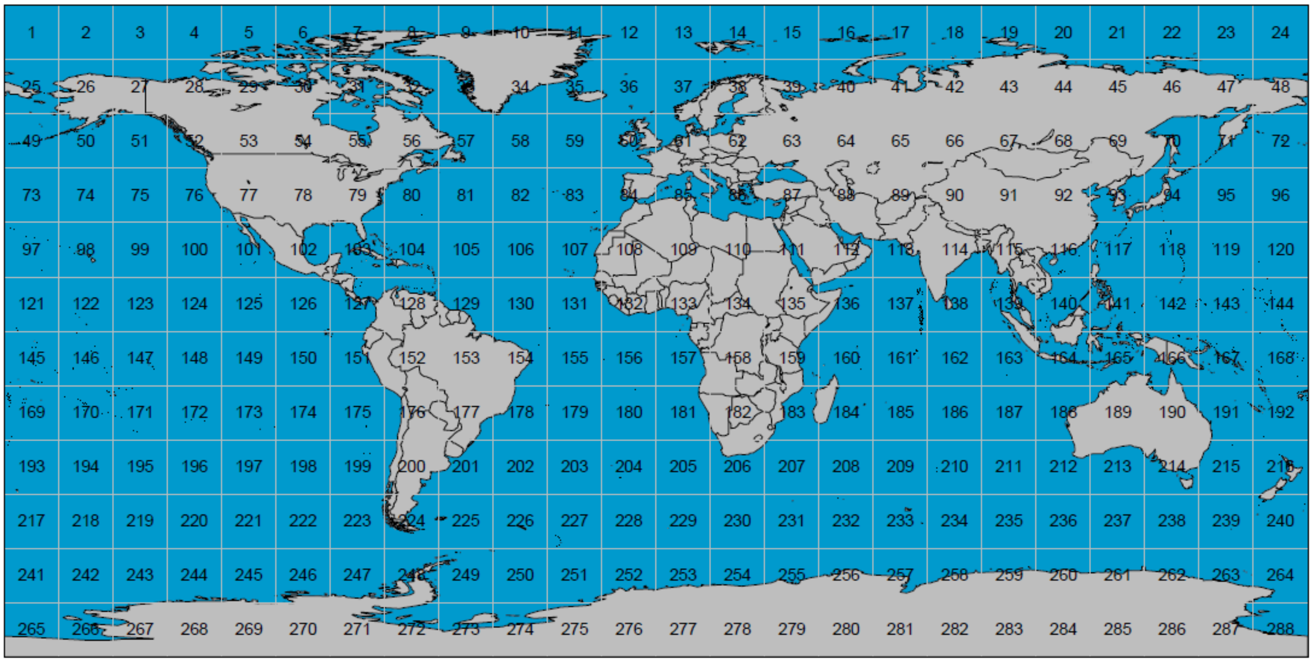

Figure 1.1. Global grid of BETR-Research at 15°×15° resolution, including nomenclature of its 288 model regions. Please note that the high resolution (3.75°×3.75°) BETR-Research has 4608 model regions.

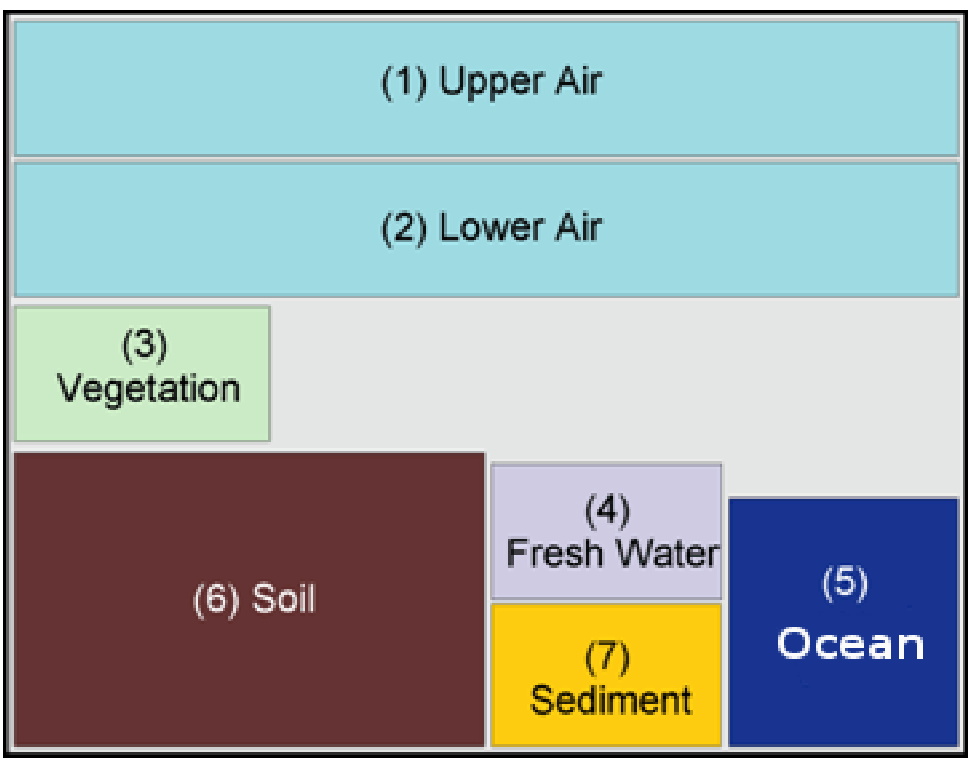

Figure 1.2. Environmental compartments included in the model regions of BETR-Research.

2. Main New Features in BETR-Research 3.0

- BETR-Research can run global model simulations in spatial resolutions of 15°×15°,7.5°×7.5° and 3.75°×3.75°.
- Environmental databases that describe global atmospheric and oceanic flows, and climate properties have been updated; and now interannual variability can be accounted for.
- Some of the chemical fate process descriptions have been modified.
- A new algorithm for tracking chemical mass transfer fluxes throughout the simulations has been added.
- A fast differential equation solver library to be used in dynamic model simulations has been integrated to the model code.
- There are options for quantifying the contribution of secondary emissions to atmospheric concentrations.

Figure 2.1 presents the schematic description of mass transfer processes between and within model regions considered in BETR-Research 3.0.

2.1. Compartment Parameterization

2.1.1. Atmosphere

Temperature fields, horizontal and vertical flows have been extracted from *ECHAM5* model output (Roeckner et al. 2003), in order to facilitate the dynamic modeling of future climate scenarios. The maybe most important improvement to the description of circulation in *BETR Research* is the calculation of vertical mixing between lower and upper atmosphere from *ECHAM5* omega levels. The previous default value of 15 m/h has been substituted by spatially and temporally resolved mixing rates. *ECHAM5* data were downloaded from the CMIP3 website (https://esg.llnl.gov:8443/home/publicHomePage.do, registered users) and the Max-Planck-Institute website (password requested).

Precipitation and runoff now stem from the *ECHAM5* model, but durations of rain events were calculated from 3-hourly precipitation data from the 20th century Reanalysis Project (Compo et al. 2011).

All atmospheric flows (vertical and horizontal) are now balanced with the limSolve package (Soetaert K. et al. 2009).

OH-radical fields data are now extracted from the *ECHAM5-HAMMOZ* model (Pozzoli et al. 2008).

2.1.2. Ocean

Skin temperature fields, horizontal and vertical flows have been extracted from *ECHAM5* model output (Marsland et al. 2003; Roeckner et al. 2003).

Ocean depth has been improved from a constant value of 100 meter to spatially and temporally resolved mixing layer depth, extracted from the BCCR-BCM 2.0 model (Bleck et al. 1992).

All oceanic flows (vertical and horizontal) are now balanced with the limSolve package (Soetaert K. et al. 2009).

Sea-ice data from the *ECHAM5* model (Marsland et al. 2003) have been introduced as a barrier that controls the fraction of total ocean area that is available for air-ocean exchange of contaminants.

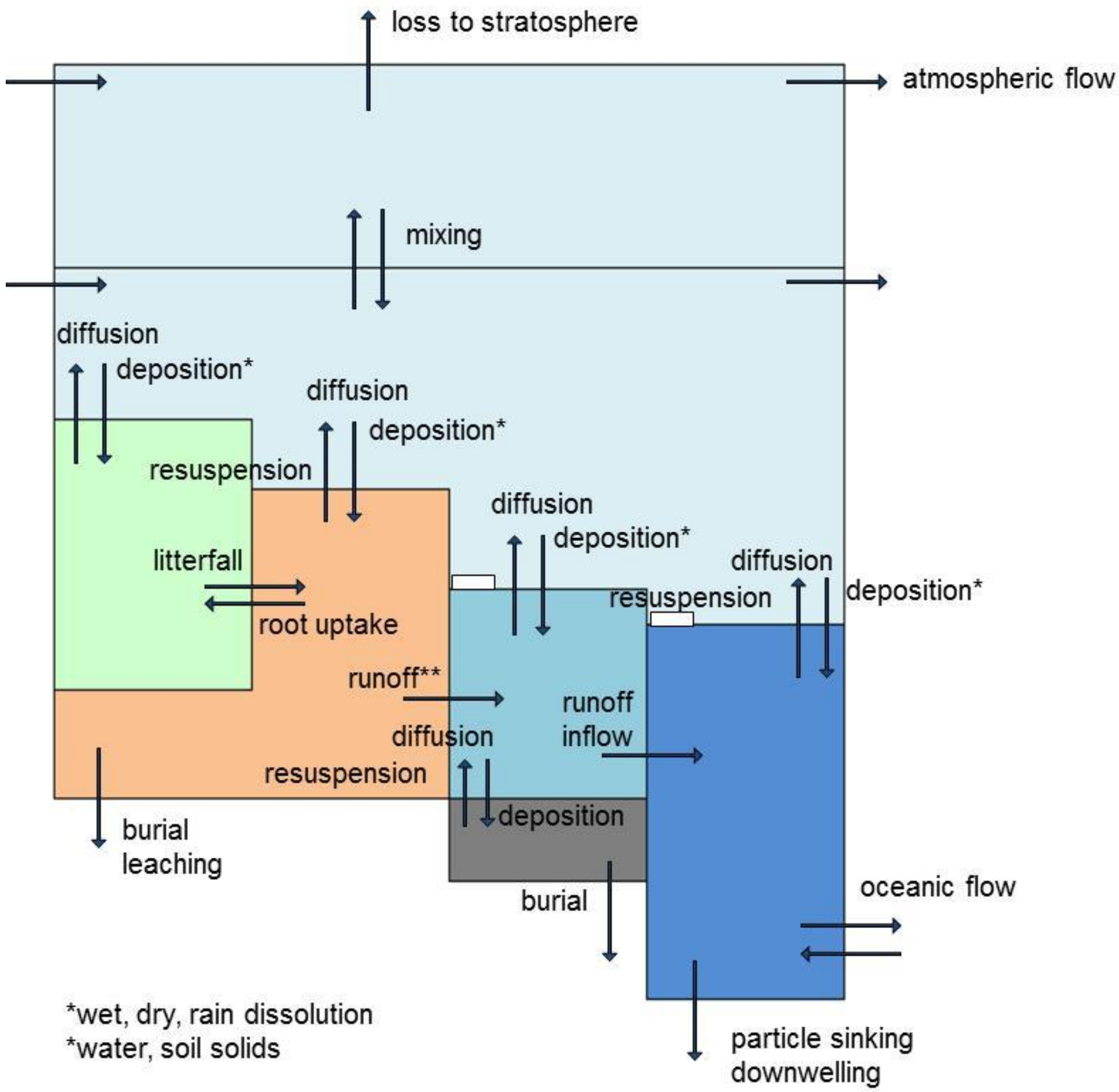

Figure 2.1. Mass transfers between and within the model regions of BETR-Research 3.0.

2.1.3. Soil

Skin temperature fields have been extracted from *ECHAM5* model output (Roeckner et al. 2003).

The content of organic carbon in soil has been extracted from the Homogenized World Soil Database (Fischer et al. 2008).

Land-ice data from the *ECHAM5* model (Marsland et al. 2003) have been introduced as a barrier that controls the fraction of total land area that is available for air-soil exchange of contaminants. Maybe the most important changes occur over Greenland.

2.1.4. Fresh Water

Fresh water surface areas have been extracted from *MODIS* satellite data (Carroll et al. 2009).

Fresh water flows have been extracted with an improved algorithm from the RivDis data base (Vörösmarty et al. 1998), eliminating some inconsistencies from the previous *BETR* parameterization.

2.2. Process parameterization

2.2.1. Partitioning between ocean/air and soil/air

In this version, sea-surface temperature and soil-skin temperature are introduced. This influences the temperature dependent partition coefficients and fugacity capacities. Also intermedia transport is influenced, insofar that the thin boundary layer above ocean and soil surface is assumed to have the same temperature as the below lying surface.

2.2.2. Leaching from soil

Leaching from soil is now calculated directly as precipitation minus runoff (from ECHAM5 data, see Section 2.1.1), and therefore spatially and temporally resolved.

2.2.3. Volatilization from soil and ocean with land- and sea-ice

The available surface for soil-air and ocean-air exchanges is reduced by the fraction which is covered by land- and sea-ice, respectively.

2.2.4. Volatilization from soil with plowing

Volatilization from soil uses now as default the volatilization algorithm for enhanced outgassing by plowing events, according to McKone et al. (2011). The time since last plowing event ('tspe') is currently implemented in the seasonal parameter file such that plowing occurs in October (March) in the Northern (Southern) hemisphere. The original algorithm without plowing enhancement will be used if the *plowingEnhance* parameter in the control-file is set to 0.

2.2.5. Option to suppress all volatilization from surface compartments to air

If the *secondarySupr* parameter in the control file is set to 1, all volatilization from surface media to air (= secondary emissions) will be suppressed. This option may be useful if *BETR* results shall be compared to results from trajectory models which do not include revolatilization (e.g. Hysplit, Flexpart).

2.3. Flux tracking

An algorithm was implemented to track mass fluxes between compartments. Sebastian Schenker did the coding using the method developed by Christine Steinlin. The code produces multiple output files that include mass transfer flux data between model compartments. Flux tracking can be switched on or off by setting the "track_fluxes" variable True or False in the run-file. This is a very useful option but it significantly increases the memory requirements.

2.4. Implementation of a fast ODE solver

A fast numerical ODE solver has been implemented. The name of the solver module is odespy. Using this module allows much faster simulations. However, we have not been able to run it on Windows. There is no problem on Linux systems. This fast solver can be switched on or off by setting the "use_odespy" variable True or False in the run-file.

2.5. Run-files

Run-files are python scripts to set up model simulations. They are meant to be used as user interfaces to the model code. Input parameters, simulation options, and output files are specified in these files. Flux tracking can be turned on or off by setting the `track_fluxes` variable `True` or `False`. Run-files also include code to track simulation time. They can be used to carry out batch-runs.

Run-files are extensively commented to guide a new user to prepare a new run.

2.6. Output

Automatically a *'summary.txt'* file is generated in which input options will be stored.

If the '*dumpDmatricesTxt*' in the control file is set to 1, an additional output file in TXT format is produced with all D-values. If only the D-matrix in TXT format is required without a model run, set the *onlybigD* parameter in the run-file to TRUE.

If the *'mkendfile'* parameter in the run-file is TRUE, then at the end of the model run, a TXT file will be generated that includes the end state of the system in moles. This file can be used as an initial-condition file for another model run.

Simulation results are written in .nc and .cpk files. The user can specify the type of output files and the desired units in the run-file. By default, these files have the prefix "OUT" followed by the name of the units used. The available units are: 'mol', 'kg', 'mol_per_m3', 'kg_per_m3', 'Pa'.

.nc files are in NetCDF format and can be viewed by using Panoply.

Flux outputs are written in .nc and .cpk files as well. They have the prefix “fluxes” followed by the description of the type of flux data they contain. The flux data is written in units of moles. These files are specified in the source code file named output.py. Currrently, the code writes many different flux output files. Unfortunately the flux output files to be written cannot be specified in the run-file. It is intended to make this possible in the near future.

2.7. Opportunities for future updates

- Implement pole disk (polar band is one single gridcell).
- Improve parameterization of the vegetation compartment, with data from MPI-ESM.
- Improve parameterization of atmospheric particles, with data from ECHAM-HAMMOZ.
- Including coastal sediment.
- Increasing vertical resolution of the atmosphere.

3. Installation

3.1. Installing the Required Software Packages

In order to run BETR-Research 3.0, a python interpreter and several add-on packages for scientifing computing are required. BETR-Research 3.0 code is written in Python version 2 and all the add-on packages should also be compatible with Python 2.

Below is a list of required software packages:

- Python version 2.7.x (Currently BETR-Research 3.0 is not compatible with Python 3)
- Numpy (version 1.11.0 or later)
- Scipy (version 0.17.0 or later)
- netCDF4 (necessary for netCDF output)
- odespy (necessary for fast dynamic simulations)
- Matplotlib (not necessary but recommended to plot results.

It is possible to install the required software packages manually. However, it is also possible to install the Python 2.7 version of **Anaconda Python Distribution**, which is an open source data science platform. When Anaconda is installed, **Python interpreter**, **Numpy**, **Scipy** and **Matplotlib** packages are installed together. Anaconda's conda tool makes it very easy to install any additional packages.

netCDF4 can be installed through conda install using the following command in the terminal window:

conda install netcdf4

odespy can be installed through anaconda.org, a repository for additional program packages. The Windows and Linux versions of odespy are found in different libraries. In Linux systems, using the following command in the terminal window will install odespy:

conda install –c undy odespy=0.3.0

For Windows systems, the following command should be used to install odespy:

```
conda install -c rothnic odespy=0.3.0
```

Using **odespy** as the differential equation solver module substantially decreases the simulation time for dynamic simulations. However, we have not been able to install and use the odespy module on Windows operating systems at the time of writing this documentation. However, it works perfectly on Linux machines

In order to easily visualize output in netCDF format, **Panoply** is recommended. Panoply is written and maintained by NASA, and can be downloaded through its website:

https://www.giss.nasa.gov/tools/panoply/

3.2. Downloading BETR-Research 3.0

After installing the required software packages, you can download BETR-Research 3.0 and start running your multimedia model simulations:

- Download BETR-Research 3.0 from the project repository on GitHub: https://github.com/rkgoktas/BETR-Research-3.0
- Unpack BETR-Research 3.0 into an arbitrary directory.
- Go over the tutorials and start experimenting with the provided example run.files.

4. TUTORIALS

Together with the source code of BETR-Research 3.0, several run-files are also distributed in order to demonstrate how to set-up different types of simulations.

Two example run-files are included for conducting global PCB simulations with BETR-Research 3.0:

run-file	Description of the simulation
run.PCB28_ivm2_corrdiffstrato_br.py	PCB28 simulation with variable annual emissions in base resolution (15°×15°)
run.PCB153_ivm2_corrdiffstrato_hr.py	PCB153 simulation with variable annual emissions in high resolution (3.75°×3.75°)

The global levels and distribution of polychlorinated biphenyls (PCBs) had previously been simulated using BETR Global (Lamon et al. 2009). In this distribution of BETR-Research 3.0, the required input parameters are provided to perform base-resolution (15°×15°) and high-resolution (3.75°×3.75°) simulations for PCB 28 and PCB 153, respectively.

The PCB emission estimates were obtained through the study of Breivik et al. (2007) that provides spatially resolved annual atmospheric emission estimates for PCBs on a 1°×1° grid up to year 2100. The emission estimate data sets were downloaded from http://www.nilu.no/projects/globalpcb/globalpcb2.htm. The emission data sets were regridded to create BETR Research emission input data sets in base resolution (15°×15°) and in high resolution (3.75°×3.75°).

The seasonal variation in the estimated emissions of PCBs were incorporated by considering the temperature dependence of the primary passive volatilization sources (main emission source) using Equation 1 in Lamon et al. (2009) which assumes that the strength of the primary passive volatilization sources is proportional to the vapor pressure of PCB congener.

The provided emission data sets are for the high emission scenario of Breivik et al. (2007) since they provide closer simulation results to the observed concentrations.

5. REFERENCES

Bleck, R., Rooth, C., Hu, D. M., and Smith, L. T. (1992). "Salinity-Driven Thermocline Transients in a Wind-Forced and Thermohaline-Forced Isopycnic Coordinate Model of the North-Atlantic." *Journal of Physical Oceanography*, 22(12), 1486-1505.

Breivik, K., Sweetman, A., Pacyna, J. M., and Jones, K. C. (2007). "Towards a global historical emission inventory for selected PCB congeners - A mass balance approach-3. An update." *Science of the Total Environment*, 377(2-3), 296-307.

Carroll, M., Townshend, J., DiMiceli, J., Noojipady, P., and Sohlberg, R. (2009). "Global raster water mask at 250 meter spatial resolution." University of Maryland, ed., College Park, Maryland.

Compo, G. P., Whitaker, J. S., Sardeshmukh, P. D., Matsui, N., Allan, R. J., Yin, X., Gleason, B. E., Vose, R. S., Rutledge, G., Bessemoulin, P., Bronnimann, S., Brunet, M., Crouthamel, R. I., Grant, A. N., Groisman, P. Y., Jones, P. D., Kruk, M. C., Kruger, A. C., Marshall, G. J., Maugeri, M., Mok, H. Y., Nordli, O., Ross, T. F., Trigo, R. M., Wang, X. L., Woodruff, S. D., and Worley, S. J. (2011). "The twentieth century reanalysis project." *Quarterly Journal of the Royal Meteorological Society*, 137(654), 1-28.

Fischer, G., Nachtergaele, F., Prieler, S., van Velthuizen, H. T., Verelst, L., and Wiberg, D. (2008). "Global Agro-ecological Zones Assessment for Agriculture (GAEZ 2008)." IIASA, FAO, Laxenburg, Austria and Rome, Italy.

Lamon, L., von Waldow, H., MacLeod, M., Scheringer, M., Marcomini, A., and Hungerbuhler, K. (2009). "Modeling the Global Levels and Distribution of Polychlorinated Biphenyls in Air under a Climate Change Scenario." *Environmental Science and Technology*, 5818-5824.

Macleod, M., Riley, W. J., and McKone, T. E. (2005). "Assessing the influence of climate variability on atmospheric concentrations of polychlorinated biphenyls using a global-scale mass balance model (BETR-global)." *Environmental Science & Technology*, 39(17), 6749-6756.

MacLeod, M., von Waldow, H., Tay, P., Armitage, J. M., Wöhrnschimmel, H., Riley, W. J., McKone, T. E., and Hungerbuhler, K. (2011). "BETR global – A geographically-explicit global-scale multimedia contaminant fate model." *Environmental Pollution*, 159(5), 1442-1445.

MacLeod, M., Woodfine, D. G., Mackay, D., McKone, T., Bennett, D., and Maddalena, R. (2001). "BETR North America: A regionally segmented multimedia contaminant fate model for North America." *Environmental Science and Pollution Research*, 8(3), 156-163.

Marsland, S. J., Haak, H., Jungclaus, J. H., Latif, M., and Roske, F. (2003). "The Max-Planck-Institute global ocean/sea ice model with orthogonal curvilinear coordinates." *Ocean Modelling*, 5(2), 91-127.

McKone, T. E., Bartelt-Hunt, S. L., Olson, M. S., and Tillman, F. D. (2011). "Mass transfer within surface soils." Handbook of Chemical Mass Transport in the Environment, L. J. Thibodeaux and D. Mackay, eds., CRC Press, Boca Raton, 159-211.

Pozzoli, L., Bey, I., Rast, S., Schultz, M. G., Stier, P., and Feichter, J. (2008). "Trace gas and aerosol interactions in the fully coupled model of aerosol-chemistry-climate ECHAM5-HAMMOZ: 1. Model description and insights from the spring 2001 TRACE-P experiment." *Journal of Geophysical Research-Atmospheres*, 113(D7).

Prevedouros, K., MacLeod, M., Jones, K. C., and Sweetman, A. J. (2004). "Modelling the fate of persistent organic pollutants in Europe: parameterisation of a gridded distribution model." *Environmental Pollution*, 128(1-2), 251-261.

Roeckner, E., Bäuml, G., Bonaventura, L., Brokopf, R., Esch, M., Giorgetta, M., Hagemann, S., Kirchner, I., Kornblueh, L., Manzini, E., Rhodin, A., Schlese, U., Schulzweida, U., and Tompkins, A. (2003). "The Atmospheric General Circulation Model ECHAM 5. Part I: Model Description." (MPI Report 349).

Soetaert K., Van den Meersche, K., and van Oevelen, D. (2009). "limSolve: Solving Linear Inverse Models. R-package version 1.5.1."

Toose, L., Woodfine, D. G., MacLeod, M., Mackay, D., and Gouin, J. (2004). "BETR-World: a geographically explicit model of chemical fate: application to transport of alpha-HCH to the Arctic." *Environmental Pollution*, 128(1-2), 223-240.

Vörösmarty, C. J., Fekete, B. M., and Tucker, B. A. (1998). "Global River Discharge, 1807-1991, Version 1.1 (RivDis)." Oak Ridge National Laboratory Distributed Active Archive Center, ed., Oak Ridge, Tennessee, U.S.A.