DOCUMENTATION of BETR-Research 3.0

Recep Kaya Göktaş

April 2017

CONTENTS:

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.

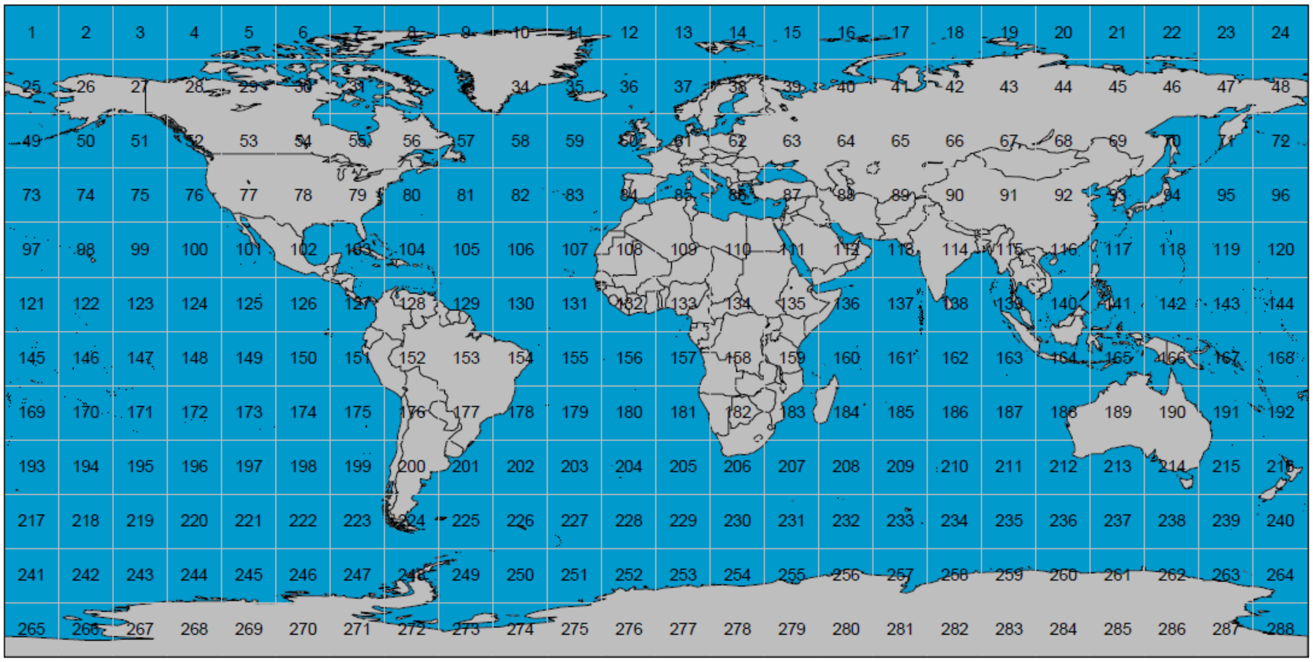

Figure 1.1. Global grid of BETR-Research at 15°×15° resolution, including nomenclature of its 288 model regions. Please note that the high resolution (3.75°×3.75°) BETR-Research has 4608 model regions.

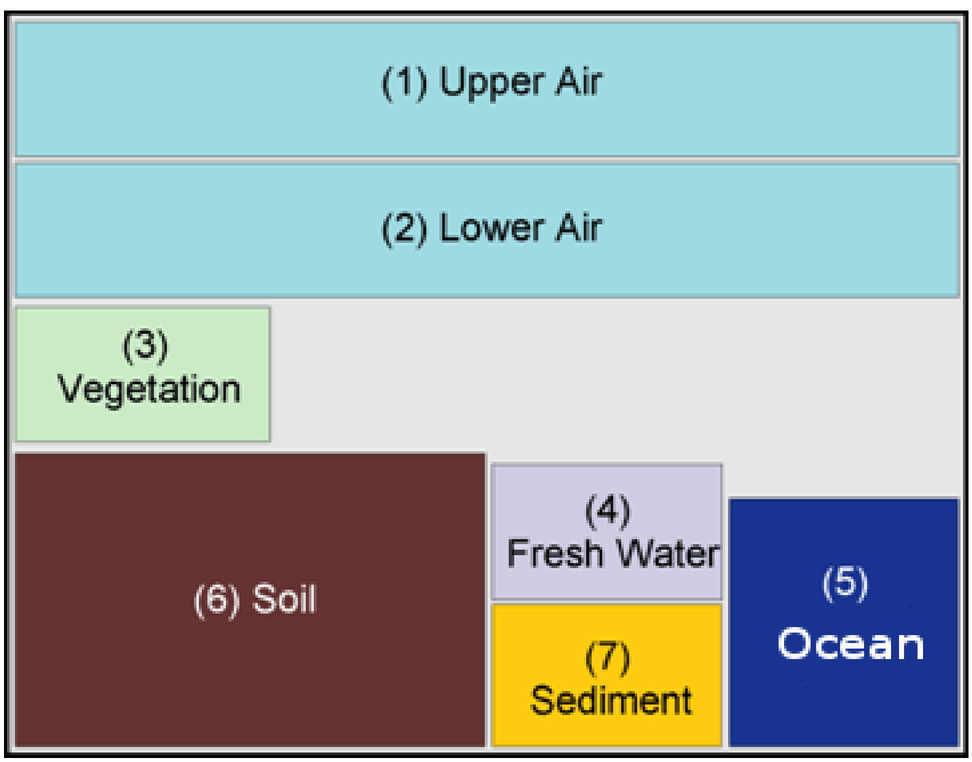

Figure 1.2. Environmental compartments included in the model regions of BETR-Research.

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 , 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 (http://www-pcmdi.llnl.gov/ipcc/about_ipcc.php) after registration, 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.

All atmospheric flows (vertical and horizontal) are now balanced with the limSolve package.

OH-radical fields data are now extracted from the *ECHAM5-HAMMOZ* model.

2.1.2. Ocean

Skin temperature fields, horizontal and vertical flows have been extracted from *ECHAM5* model output.

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.

All oceanic flows (vertical and horizontal) are now balanced with the limSolve package .

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

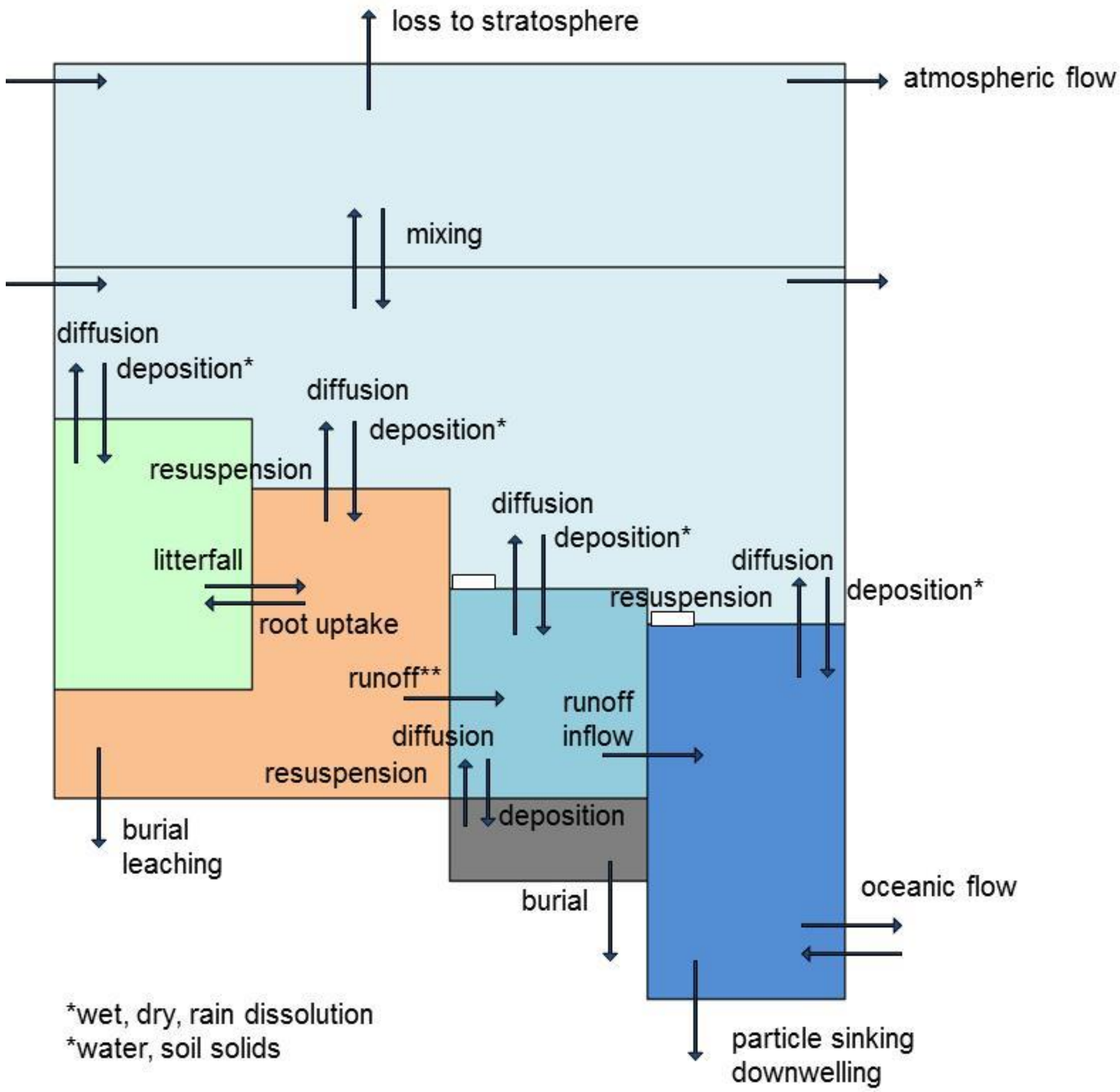

Figure 2.1. Mass transfers between and within the model regions of BETR-Research 3.0.

2.1.3. Soil

Skin temperature fields have been extracted from *ECHAM5* model output.

The content of organic carbon in soil has been extracted from the Homogenized World Soil Database.

Land-ice data from the *ECHAM5* model 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.

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

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. REFERENCES

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.

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.

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.