Global-Scale Multimedia Chemical Fate Modeling in High Spatial Resolution: Introducing BETR-Research 3.0

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The family of BERKELEY-TRENT (BETR) Multimedia Fate Models

BETR-Research 3.0 is the newest member of the BETR family of spatially explicit multimedia fate and transport models:

- 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)**

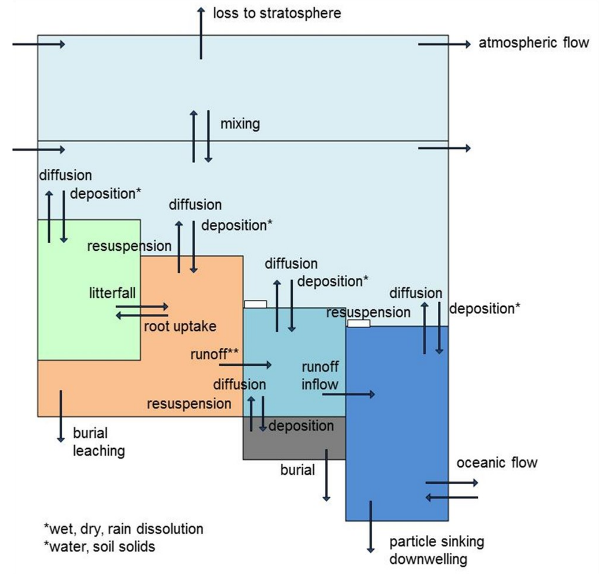

Figure 1: Mass transfers between and within the model regions of *BETR-Research 3.0*.

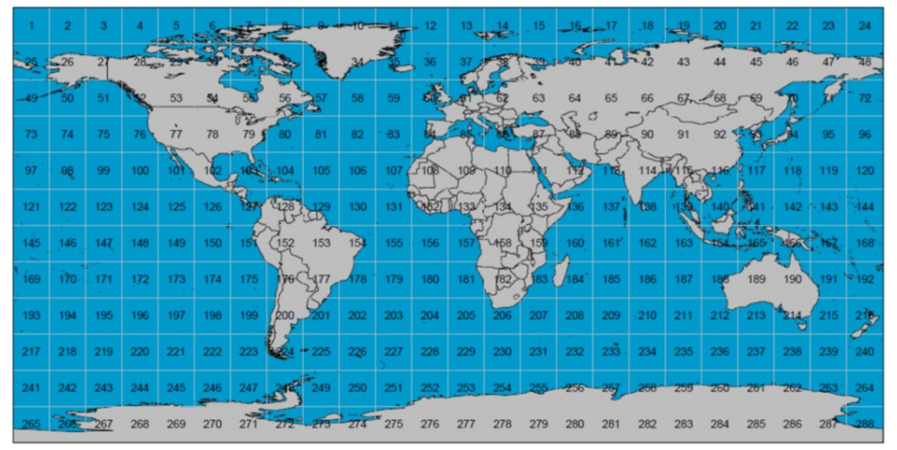

Figure 2: Global grid of *BETR-Research* at 15°×15° resolution, including nomenclature of its 288 model regions. Please note that the high-resolution (3.75°×3.75°) *BETR-Research 3.0* has 4608 model regions.

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.

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

Main New Features in *BETR-Research 3.0*

- *BETR-Research 3.0* 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.

OBJECTIVE

We demonstrate *BETR-Research 3.0* by simulating the global distribution of two polychlorinated biphenyls (**PCB28** and **PCB153**).

This model application was used to verify the implementation and new process descriptions in the new version, and to establish that the **high-resolution environmental data set** is reliable for use in future *BETR-Research* global modeling studies.

Global-Scale Multimedia Chemical Fate Modeling in High Spatial Resolution

The global distribution of PCB28 and PCB153 have been simulated by *BETR-Research 3.0* in 3.75°×3.75° spatial resolution. This application is a high-resolution upgrade of a previous modeling study using BETR-Global (Lamon et al. 2009).

The PCB emission estimates were obtained through Breivik et al.'s (2007) study that provides spatially resolved annual atmospheric emission estimates for PCBs on a 1°×1° grid between 1930 and 2100. The emission estimate data sets were downloaded from http://www.nilu.no/projects/globalpcb/globalpcb2.htm.

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) by assuming that the strength of the primary passive volatilization sources is proportional to the vapor pressure of the PCB congener (Lamon et al., 2009).

PCB153 emissions in 2012

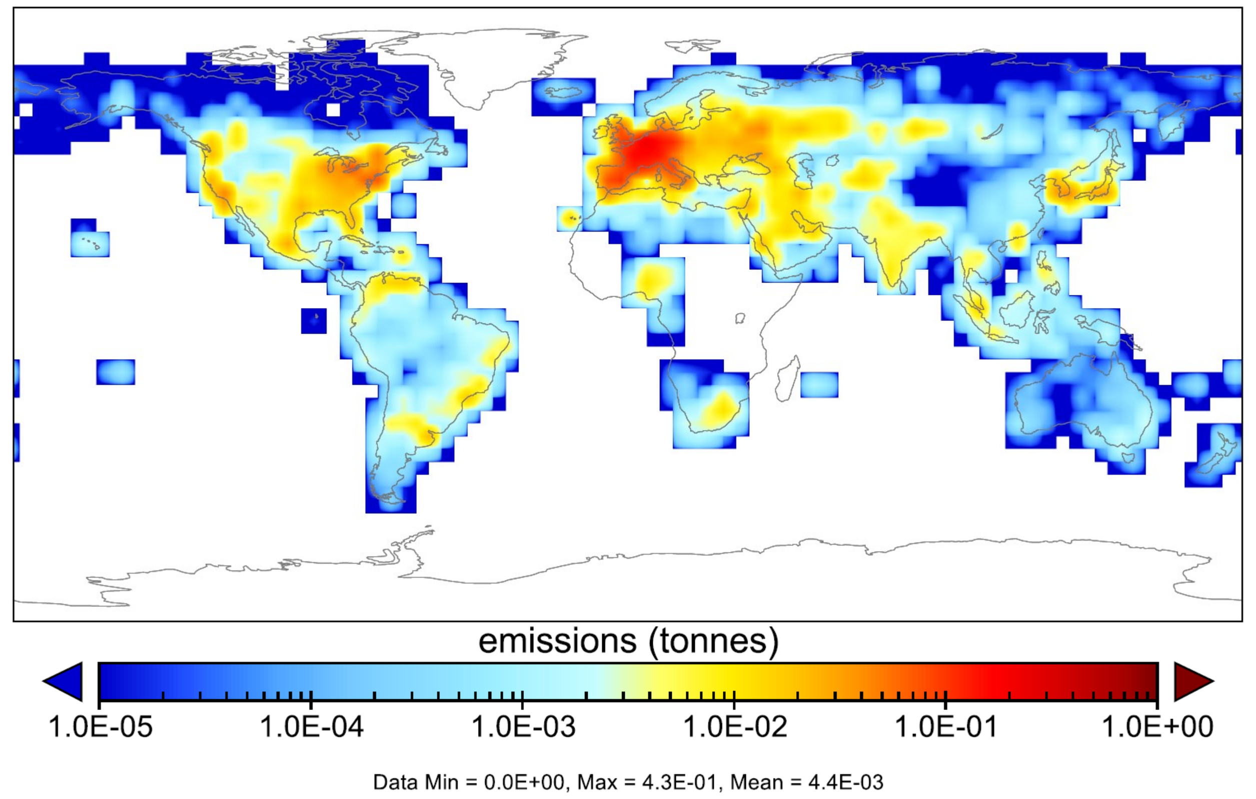

Figure 3: Annual PCB153 emissions in each model region (3.75°×3.75° grid) of *BETR Research 3.0* for the year 2012. Emission estimates are for the Maximum Scenario in Breivik et al. (2007), which was also used in the model simulations.

ACKNOWLEDGEMENTS

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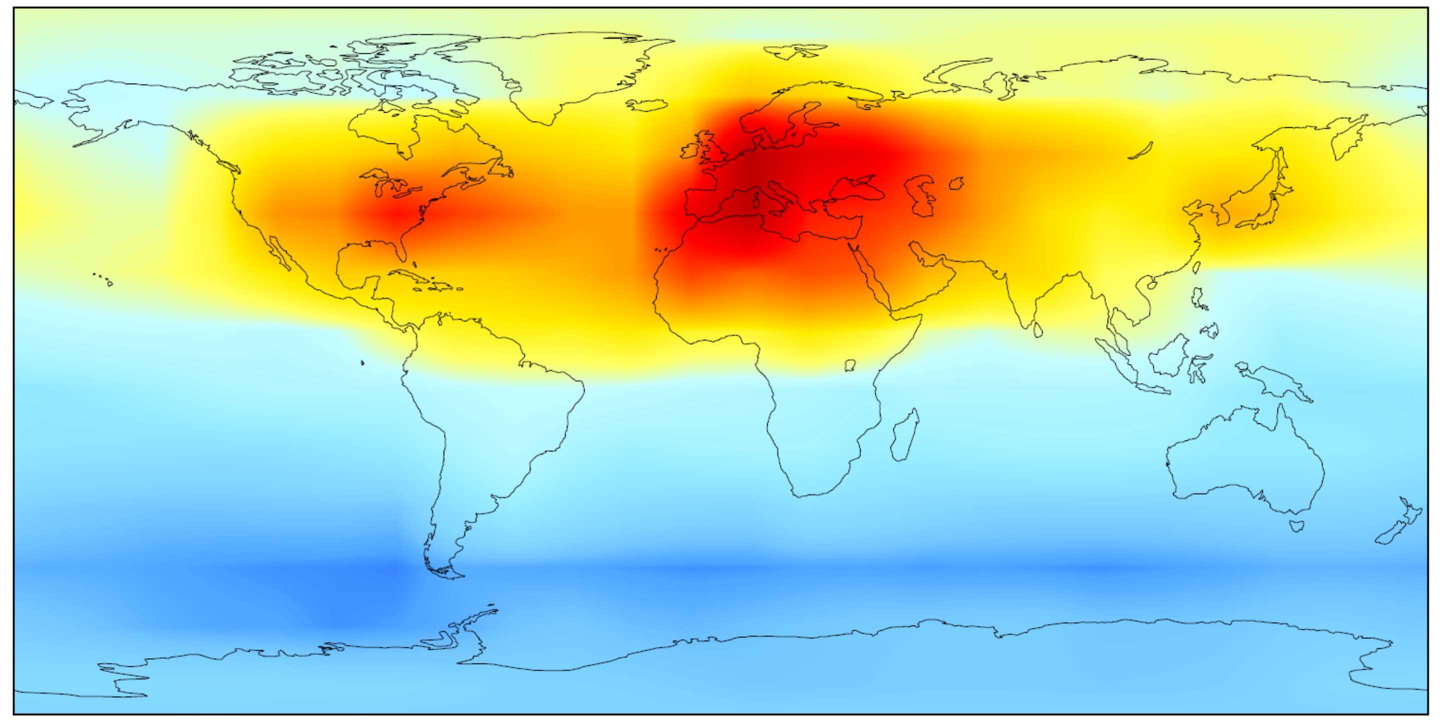
Comparison of Base Resolution and High Resolution Simulation Results

PCB153 Concentrations in Lower Air (July 2012)

A) Base Resolution (15°×15°)



B) High Resolution (3.75°×3.75°)

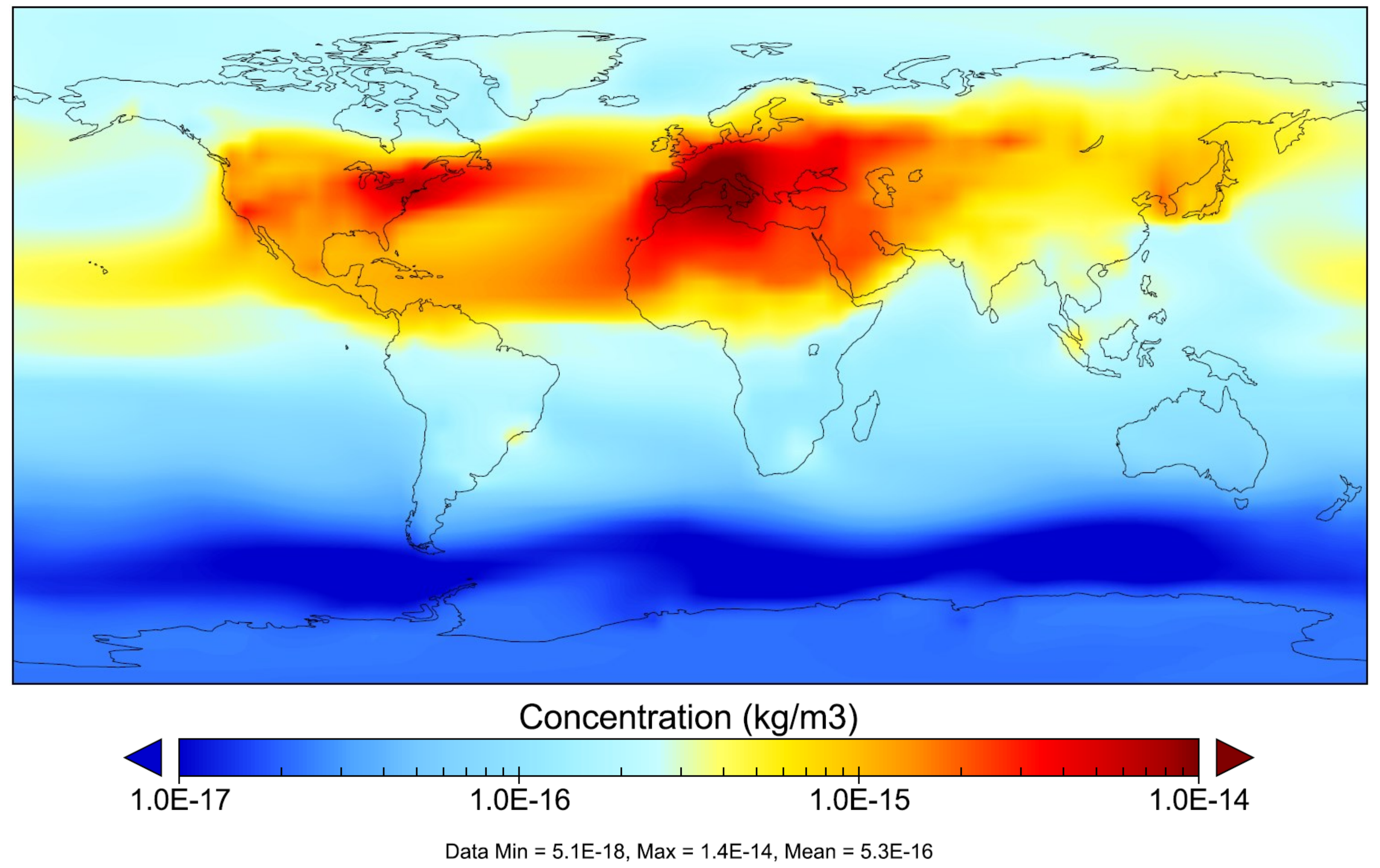


Figure 4: Comparison of *BETR-Research 3.0* simulation results for PCB153 concentrations in lower air for the year 2012, in (A) base, and (B) high spatial resolutions.

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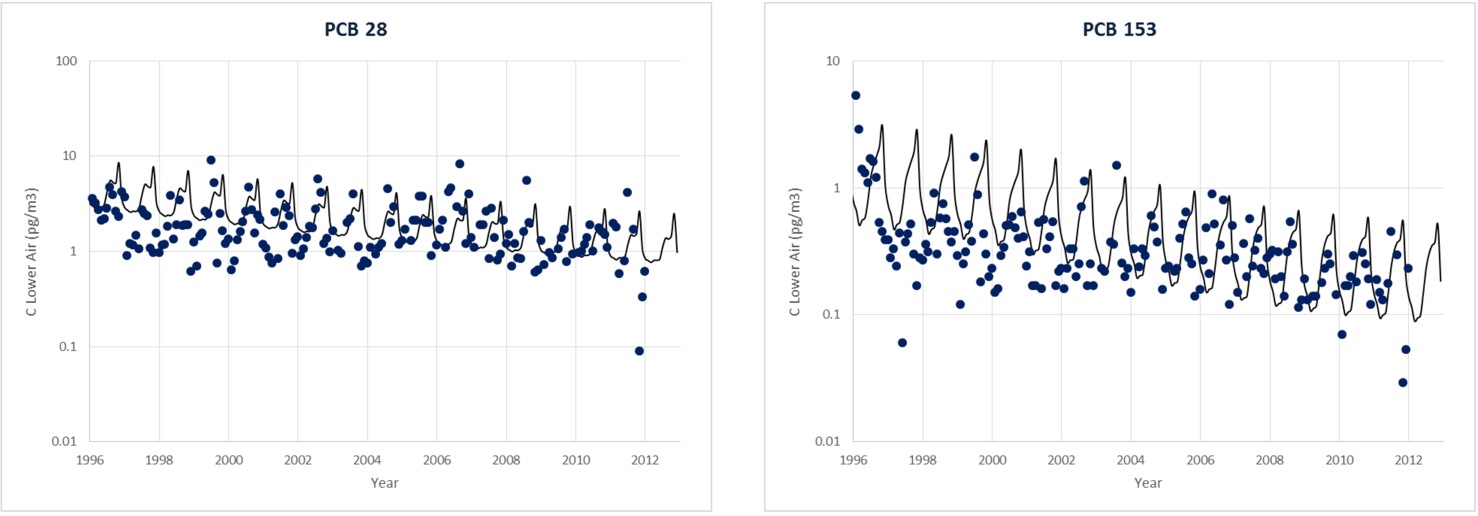
High Spatial Resolution Results and Comparison with Observations

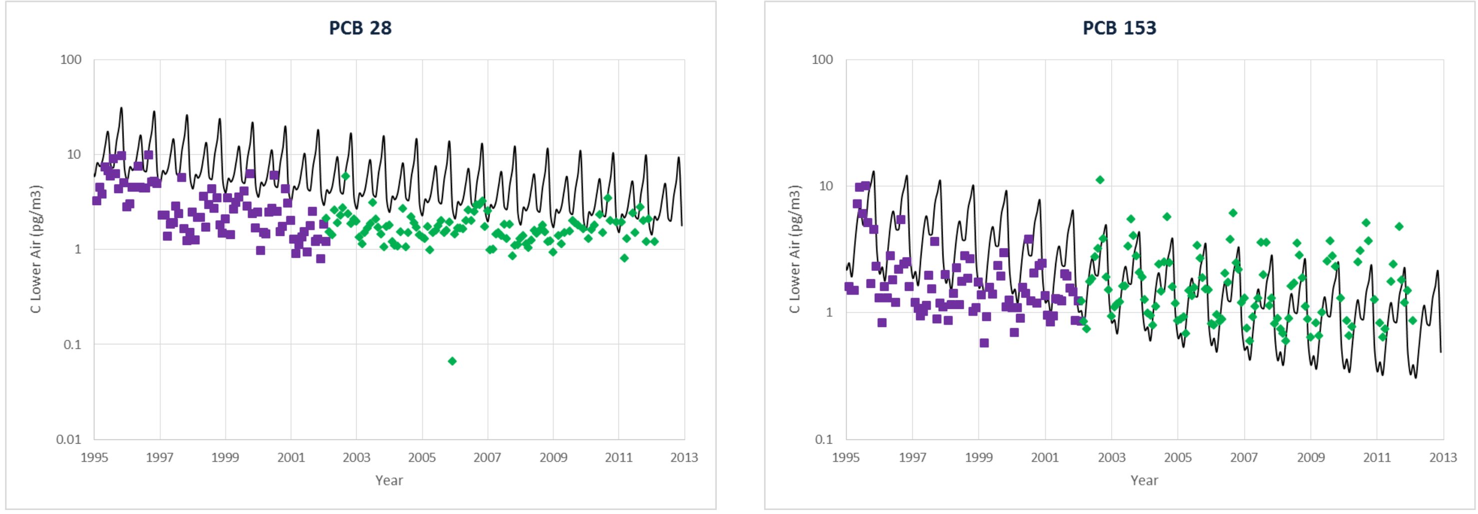
Observed PCB data sets were compiled from the following sources:

- EBAS database (operated by Norvegian Institute for Air Research) (ebas.nilu.no)
- IADN (Integrated Atmospheric Deposition Network, Environment Canada)
- IVL (Swedish Environmental Research Institute)

Pallas, Finland



Rörvik, Sweden & Rao, Sweden



Burnt Island, Canada

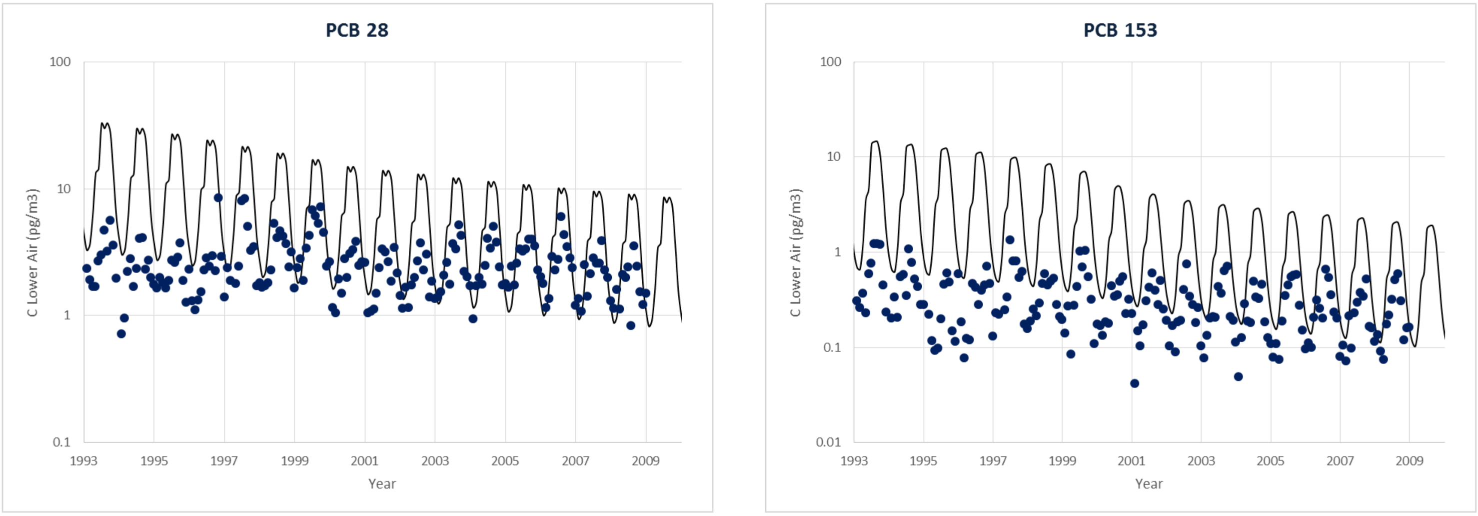


Figure 5: Comparison of the high-resolution simulation results with the observed concentrations at selected monitoring stations throughout the globe.

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