Enhanced BETR Global Release and Evaluation Against PMCAMx

Fangyuan Zhao, Ilona Riipinen and Matthew MacLeod

Stockholm University, Department of Environmental Science, Stockholm, Sweden

May 7, 2020

Work Package 4 – Integrating in-situ, satellite and model components for improved environmental assessment

Task 4.4 – Impact assessment and future exposure scenarios of pollutants in the Arctic

Deliverable 4.4.1 – Enhanced PMCAMx and BETR Global Ready

Version RC002

Enhanced BETR Global ready

A steady-state mass balance method for predicting gas-particle concentration ratios of organic chemicals was validated in a regional model (see Deliverable 4.4.1 - Report on Enhanced Modeling Capabilities for POPs). We have now implement this method in BETR Global as BETR Global 4.0 that has been uploaded on the open source code repository Github https://github.com/BETR-Global/BETR-Global-4.0. The enhanced version of BETR Global (v. 4.0) is thus publically available from the website for use according to the accompanying user's guide document.

Important new features in BETR Global 4.0:

- The number of compartments in each region is increased to 10 by including the coarse particle compartment in upper air, fine particle compartment in lower air and coarse particle compartment in lower air.
- Emissions of chemicals can be as gas phase, fine particle and coarse particle phases.
- Environmental parameters including fraction of organic matter in particles, volume fractions of particles, velocities of particles and diameters of particles are different in each cell. Values are decided by the aerosols' type. Aerosols' types are the same with them in the regional model, which are seven scenarios including urban, rural, remote, marine, free troposphere, polar and desert.

Plans for the future work:

- Calculate concentrations of low volatility chemicals such as BDE209 at a global scale with BETR Global 4.0. Then make comparisons with 1) the old versions of BETR Global 2) and measurements.

- Calculate gas-particle concentration ratios of low volatile chemical at a global scale with BETR Global 4.0. Then make a comparison with measurements.
- Combine BETR Global 4.0 with ACC-HUMAN model to predict exposure of humans to chemicals at a global scale (for Deliverable 4.4.2, which is anticipated at the end of June).

Evaluation of BETR global with results obtained using PMCAMx

After the beginning of the project it became evident that fully updating two pollutant transport models (namely BETR Global and PMCAMx) for the inclusion of the environmental pollutants targeted within iCUPE would be somewhat redundant. Instead, we decided to focus the effort on developing the process modeling capacities of BETR Global and to evaluate the approach using the detailed aerosol particle fields produced by PMCAMx in previous studies (e.g. Fountoukis et al., 2011[1] and Megaritis et al., 2013[2]).

The sensitivity studies conducted with the process model that we used to improve BETR Global (Zhao et al., *to be resubmitted to Environ. Sci. Technol.*) indicated that the key parameters that influenced the gas-particle concentration ratios and transport of semi- and low-volatile chemicals were on one hand the properties assumed for the chemicals, and on the other hand the properties of the aerosol size distribution, in particular the mass loading and average size. To investigate the representativeness of the seven scenarios incorporated in BETR Global 4.0, we made a comparison of the aerosol fields simulated by the PMCAMx and the scenarios assumed within BETR Global 4.0. In particular, we compared of the fraction of organic matter in aerosols and volume fraction of aerosols in air (see Table 1), since these were identified as key parameters in our sensitivity analysis.

Summary of results from Table 1:

- Fractions of organic matter in coarse aerosols in BETR Global 4.0 are generally consistent with values simulated by PMCAMx in the European domain (free troposphere and desert were excluded from this comparison). In marine and polar cases, fraction of organic matter in fine aerosols are also consistent, while values in BETR are somewhat higher than they are in PMCAMx in urban, rural and remote areas. The exact reasons for this discrepancy are unclear but might be related to the details of e.g. semi- and low-volatile condensation onto the fine particle fraction.[3]

- Volume fraction of fine aerosol in BETR Global 4.0 and PMCAMx are within the same order of magnitude in urban, marine, rural, remote and polar, while volume fraction of coarse aerosols are within an order of magnitude in those scenarios.

In brief, we deem the agreement between the simplified scenarios and the detailed aerosol model (PMCAMx) acceptable to move forward with the application of these scenarios within the planned BETR Global scenarios for low volatility chemicals.

Table 1. f_{OM} is the fraction of organic matter in aerosol particles. V_P/V_A is the volume fraction of aerosol particles in air. F and C are fine and coarse aerosols.

		f_{OM}		V_P/V_A	
		BETR	PMCAMx	BETR[4]	PMCAMx
Urban	F	0.8[5]	(0.35-0.55)[1] 0.36[6]	3.64E-11	2.1E-11[6]
	C	0.23[5]	0.21[7] 0.42[6] 0.5[8]	4.82E-11	1.34E-11[9] 1.07E-11[7] 6.7E-11[8]
Marine	F	0.1[10]	(0.15-0.25)[1]	2.04E-12	1.68E-12[1]
	C	0.05[10]	0.08[2]	1.39E-11	5.02e-12[2]
Rural	F	0.8[5]	(0.35-0.55)[1]	4.53E-12	4.2E-12[1]
	C	0.23[5]	0.27[7] 0.32[8]	1.73E-11	8.35E-12[2] 7.6E-12[7] 5.36e-12[8]
Remote	F	0.8[5]	(0.35-0.55)[1]	7.31E-12	4.2E-12[1]
	C	0.23[5]	0.32[8]	2.53E-11	8.35E-12[2] 5.36e-12[8]
Free Troposphere	C	0.2[10]	_	6.07E-14	_
Polar (clean)	F	0.3[a]	(0.25-0.37)[1]	1.4E-13	6.7E-13[1]
	C	0.1[a]	0.1[2]	8.89E-13	4.36E-12[2]
Desert	C	0.05[a]	_	1.77E-09	_

a: values are estimated.