Towards a Nested Exposure Model for organic contaminants (NEM)

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Introduction

Most environmental monitoring programs on organic contaminants, such as persistent organic pollutants (POPs), have a restricted explicit geographical scope, targeting a specific country or region. Such programs often aim to support relevant policy efforts, allowing for evaluation of empirical trends, which may be further explored in concert with mathematical models to allow for a better understanding of the link between sources and environmental exposures in a given region of interest. Hence, there is typically both regulatory and scientific interest to better understand and potentially predict how source-exposure relationships may vary in space and time, for individual contaminants and across abiotic and biotic compartments. As POPs are recognized as global pollutants because of their known potential for long-range environmental transport, sources affecting a specific region could both be distant and/or of more local origin. Furthermore, the persistence of POPs implies that current exposures could be a result of both historical as well as recent emissions. This calls for regional modelling strategies that are global in context, yet dynamic, reflecting both the possible mobility and lifetime of relevant contaminants in the physical environment and in the human food-chain. Here, we introduce the initial version of an integrated Nested Exposure Model (NEM). NEM reflects the hypothesis that accurate predictions of organic contaminant exposures call for increasing resolution with increasing proximity to a study region of specific interest.

Materials and methods

The point of departure for NEM are three existing dynamic (time-variant) fugacity-based multimedia models (*1*), notably BETR-Global (*2*), ACC-Human (*3*) and CoZMo-POP 2 (*4*). In brief, both the BETR-Global and CoZMo-POP 2 model are organic contaminant fate models of the physical environment containing multiple environmental compartments. However, a key distinction is that CoZMo-POP 2 is a non-spatially resolved model whereas BETR-Global is a gridded spatially-explicit global-scale model. Within NEM, the processes described within individual grid cells largely reflect CoZMo-POP 2, while the transport of chemicals from one grid to the other are based on BETR-Global. ACC-Human, in contrast is a food-chain bioaccumulation model containing both a simple pelagic food-chain and a terrestrial food-chain with human as the top predator, and which may be added to a user-defined grid cell of specific interest. We refer to the original publications for details.

In contrast to the models mentioned above, the NEM model is being developed as a nested model (Figure 1).

Through nesting different model domains, NEM offers increasing resolution with increasing proximity (in space and time) to a given study region of interest. To illustrate the utility of the model we have selected the Nordic region, including remote Arctic areas such as Svalbard, as an initial case study. However, the NEM model is developed such that any other region may be targeted in a similar fashion. The Nordic region was chosen as it is probably among the more intensively studied regions with respect to the empirical occurrence of organic contaminants within various ecosystems, making it a suitable region for model evaluation. The regions is also interesting for the purpose of testing the model as it likely contains areas impacted by local emissions as well as areas assumed predominantly influenced by long-range environmental transport. For this example, the initial version of NEM allows for simulation of (up to) five different gridded model domains, simulated in sequence: Global (30ºx120º Latitude/Longitude) > Northern Hemisphere (30ºx30º) > "Europe" (15ºx15º: 30ºN to 90ºN, -30ºE to 60ºE) > "Northern Europe" (7.5ºx7.5º: 45ºN to 90ºN, -7.5ºE to 37.5ºE) > "Nordic region" (3.75ºx3.75º: 52º30'N to 75ºN, 0ºE to 30ºE). Chemical transport between neighboring grid cells may occur by air, fresh water and seawater, which in turn is parameterized on the basis of the high-resolution version (3.75ºx3.75º) of BETR-Global (*5*). From sequential simulations, chemical inflow from the outside world and into the next domain of NEM (except the initial global domain), is based on model outputs from simulations of the preceding domain.

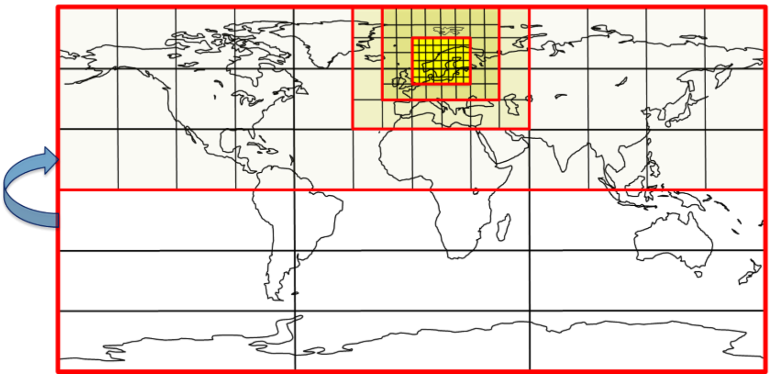

Figure 1. *Nested model domains (red boxes) explored in the simulations presented: Global (30°x120° Lat/Long) > N. Hemisphere (30°x30°) > Europe (15°x15°) > N. Europe (7.5°x7.5°) > Nordic region (3.75°x3.75°).*

The NEM model is developed from the code of CoZMoMAN (*6*) which is a linked version of ACC-Human and CoZMo-POP 2. The physical environment of each grid cell within NEM includes up to 10 different compartments (upper and lower atmosphere, broadleaf and needleleaf canopies, forest soil, uncultivated soil, agricultural soil, fresh water, fresh water sediment and marine water). While BETR Global includes one soil compartment, NEM includes up to three (forest soil, uncultivated soil and agricultural soil). The forest soil compartment is in turn covered by one or two canopy compartments (coniferous canopy and/or broadleaf canopy). The surface areas for each terrestrial compartment in NEM are based on data on various land cover classes from the International Geosphere-Biosphere Programme IGBP (*7*). First, data for each IGBP land cover class was lumped to match the spatial resolution at 3.75ºx3.75º. The forest soil area within each grid cell was set equal to the sum of the areas for needle-leaf forests (evergreen + deciduous), broadleaf forests (evergreen + deciduous) and mixed forests. The surface areas for each needle-leaf and broadleaf forest canopy compartment were estimated on a similar basis. Agricultural soil areas in NEM were assumed equal to the area of the IGBP category cropland plus half of the area for the IGBP category referred to as cropland/natural vegetation mosaic. Finally, the areas for the uncultivated soil compartment were assumed equal to the total area of any other IGBP terrestrial land cover class. The fraction of each soil compartment within each grid cell was then derived and multiplied by the BETR-Global soil areas to ensure consistency with the original parameterization. The NEM model additionally includes the opportunity to simulate bioaccumulation in the human food-chain within a user-defined grid cell, allowing predictions of both abiotic and biotic exposures (Figure 2). The NEM model was run for PCB-153 from 1930 until present time, using a global historical emission scenario (*8*) and chemical property data from references listed in Breivik et al (*6*) as model input.

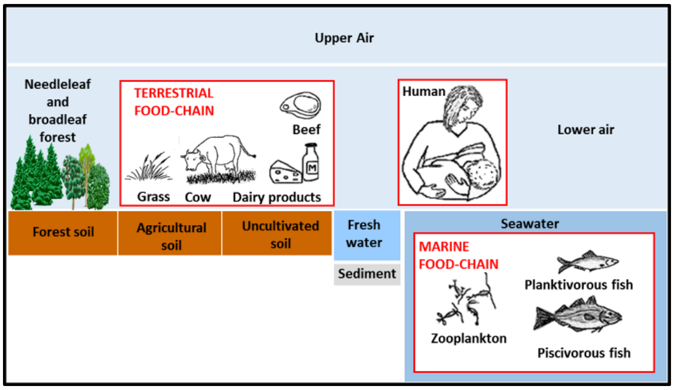

Figure 2: *Abiotic and possible biotic compartments within a given grid cell within in NEM (modified after Breivik et al (6)).*

Results and discussion

The NEM model is still under development. Results are therefore preliminary and intend to illustrate the potential future utility of NEM only. We have selected lower air as an example to illustrate model outputs (Figure 3). Predicted and observed long-term temporal trends from various EMEP and AMAP air monitoring stations are additionally included. Through further research, we will seek opportunities to (*i*) further improve and refine the model in terms of both resolution and realism, (*ii*) expand the food-chain to include additional wildlife species, and (*iii*) critically confront model predictions with observations (for additional media and contaminants). In the longer run, we hope the nested model may serve as a useful tool to help understand and predict source-exposure relationships in specific regions, which complements and expand on the models for which it is based. We believe the nested model may be particularly useful in comparison to non-spatially resolved models when the key interest is on targeting a specific region for which exposures may be significantly affected by inflow of chemical from the outside world. Secondly, as a given target region is captured in any domain simulated, NEM also allows for evaluation of the impact of variable spatial resolutions on predicted exposures in the region of interest.

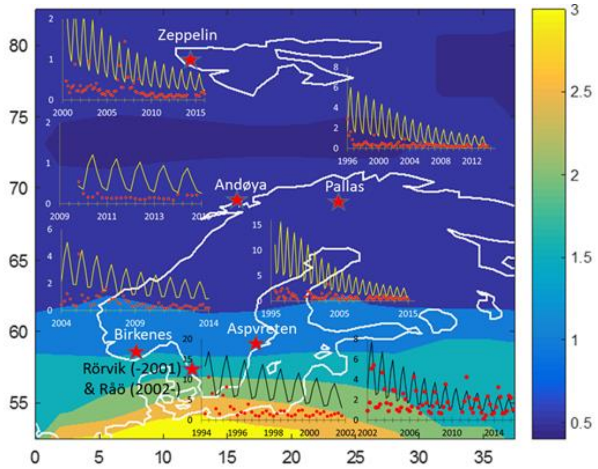

Figure 3: *The map shows the predicted spatial pattern of PCB-153 in lower air in spring 2006. We have included an illustrative comparison of predicted (line) and observed (red dots) seasonally-averaged long-term temporal trends for monitoring sites in the study region (ebas.nilu.no). Unit is pg/m^3.*

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