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Development of a multimedia model (POPsLTEA) to assess the influence of climate change on the fate and transport of polycyclic aromatic hydrocarbons in East Asia

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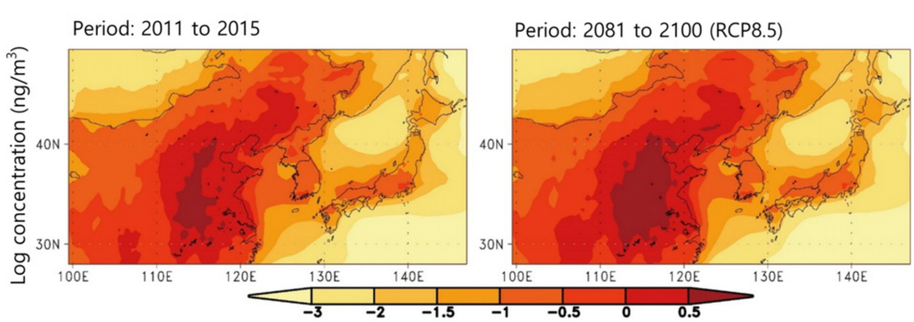
HIGHLIGHTS

- A multimedia model (POPsLTEA) assesses climate change influence in East Asia.
- POPsLTEA was evaluated by comparing against multimedia monitoring data.
- POPsLTEA is applicable to semi-volatile organics including POPs and PAHs.
- A case of benzo(*a*)pyrene is presented in the multimedia environment under RCP8.5.

GRAPHICAL ABSTRACT



Change in the atmospheric concentration of benzo(*a*)pyrene predicted using POPsLTEA

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ABSTRACT

A dynamic multimedia model (POPsLTEA) for an East Asia region was developed and evaluated to quantitatively assess how climate change (CC) alters the environmental fate and transport dynamics of 16 polycyclic aromatic hydrocarbons (PAHs) in air, water, soil, and sediment. To cover the entire model domain (25°N–50°N and 98°E–148°E) where China, Japan, and South and North Koreas are of primary concern, a total of 5000 main cells of 50 km × 50 km size were used while 1008 cells of a finer spatial resolution (12.5 km × 12.5 km) was nested for South Korea (33°N–38°N and 126°E–132°E). Most of the predicted concentrations agreed with the observed values within one order of magnitude with a tendency of overestimation for air and sediment. Prediction of the atmospheric concentration was statistically significant in both coincidence and association, suggesting the model's potential to successfully predict the fate and transport of the PAHs as influenced by CC. An example study of benzo(*a*)pyrene demonstrates that direction and strength of the CC influence on the pollution levels vary with the location and environmental media. As compared to the five year period of 2011 to 2015, the changes across the model domain in the annual geometric mean concentration over the years of 2021 through 2100 were predicted to range from 88% to 304%, from 84% to 109%, from 32% to 362%, and from 49% to 303%, in air, soil, surface water, and sea water, respectively, under the scenario of RCP8.5.

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1. Introduction

It is generally acknowledged that climate change (CC) can influence every step along the fate, transport, and distribution pathways of chemicals in the environment (Gusev et al., 2012; Dalla et al., 2007). Semi-volatile organic chemicals (SVOCs) including polycyclic aromatic hydrocarbons (PAHs) and persistent organic pollutants are of particular concern because CC can readily impact the quality of multiple environmental media because of the compounds' cross-media characteristics (Kallenborn et al., 2012; Teran et al., 2012; Schiedek et al., 2007).

The number of studies exploring the influence of CC on environmental fate and transport of pollutants seems to be growing (Marquès et al., 2016; Hansen et al., 2015; Nadal et al., 2015; Cai et al., 2014; Kallenborn et al., 2012; Noyes et al., 2009; Macdonald et al., 2003). Previous studies often addressed effects of individual climate parameters (Noyes et al., 2009; Dalla et al., 2007; Schiedek et al., 2007; Wania and Daly, 2002) and/or effects on a pollution level in a single medium (Amell et al., 2015; Harley et al., 2006; Macdonald et al., 2003) In these studies, the complicated and interdependent natures among the parameters and/or the environmental media were generally left out. Also, quantitative assessment of the CC influence has been limited (Balbus et al., 2013; Lamon et al., 2009a; MacLeod et al., 2005; Dalla et al., 2003).

To overcome these limitations, multimedia models may serve as an excellent tool which can assess the CC influence in quantitative and integrated manners on the pollution level in multiple environmental media. Macleod et al. (2005) and Earnshaw et al. (2015) predicted by using a level III multimedia model the pollution distribution of polychlorinated biphenyls (PCBs) and polybrominated diphenyl ethers (PBDEs) as influenced by the weather change for a period of 50 years at global and European scales. Also, Globo-POP (Wania and Mackay, 1999) was used to analyze the importance of hydroxyl radical (Wania and Daly, 2002) and temperature (Wania, 2003) to the transport of PCBs while BETR-Global (Macleod et al., 2001, 2005) was used to predict that higher temperature under a climate change scenario causes increase in the atmospheric concentration of PCBs (Lamon et al., 2009b). Zhu et al. (2014) demonstrated using SESAMe that potential long-range transport of pollutants can change significantly with a change in wind speed in China.

According to the study objectives, however, these previous studies used multimedia models that adopt assumptions of equilibrium among the environmental compartments and/or steady state with which dynamic nature of the CC influences cannot be readily captured. Also, the pollutants of concern in the model studies were limited to typical persistent organic pollutants such as PCBs and PCDDs/DFs (Nadal et al., 2015).

Long range transport of pollutants among East Asian countries has already been an important issue including SOx (Wang et al., 2008), sulfate and nitrate (Fairlie et al., 2010), heavy metals (Kusunoki et al., 2012), and polybrominated biphenyls (Law et al., 2014). With growing industrialization and economy in these countries, more number of hazardous substances are likely to be emitted with increasing quantity, which will add to the significance of the long range transport issues. Besides, quantitative understanding of the impacts of CC on the long range transport is critical to managing the future environmental quality of this region. However, existing modeling studies focused mostly on Europe or the globe (MacLeod et al., 2011; Hauck et al., 2008) while only a few studies have been conducted on CC influence in the multimedia environment which are limited to individual countries such as China (Liu et al., 2014) and South Korea (Cai et al., 2014). In the absence of an adequate multimedia model to address issues of long range transport of various SVOCs including persistent organic pollutants (POPs) and PAHs, we developed a dynamic multimedia fate and transport model (Persistent Organic Pollutants Long Range Transport model for East Asia, POPsLTEA) for an East Asia region aiming to quantitatively assess how the long range transport dynamics in the multimedia environment vary with climate change. In the present work, the development of POPsLTEA and its evaluation results for the 16 PAHs were presented. The PAHs from pyrogenic sources (Lee et al., 2004) were selected because many of them possess POPs characteristics (OSPAR) and they are ubiquitous pollutants of great environmental concern (Tobiszewski and Namiesnik, 2012) and their atmospheric emission will continue in the region.

2. Materials and methods

2.1. Climate change scenario

Meteorological data used in this study comprised of reanalysis data based on the observation and predicted data under the RCP8.5 scenario for the periods from 1956 to 2005 and from 2006 to 2100, respectively. The RCP8.5 data were produced by HadGEM2-AO (Jones et al., 2011; Stott et al., 2006) developed in the Coupled Model Inter-comparison Project (CMIP5) with the horizontal resolution of 135 km × 135 km. The resolution was then scaled down for 50 km × 50 km and 12.5 km × 12.5 km for the East Asia and South Korea (NIMR, 2011), respectively. Need of the finer resolution for South Korea was recognized in the model design phase for more detailed analysis. The data indicates that temperature in the study area rises by about 7 °C over the 145 years (1956 to 2100) (Fig. 1(a)), which is greater than the global average of 3.7 ± 0.74 °C (NIMR, 2012). The annual average temperature and the precipitation is statistically not the same among the three countries and sea while the increasing rates in temperature and precipitation with time shows no statistical difference (Levene and Dunnett T3 tests). It was notable that fluctuation in the annual precipitation is greater in South Korea than in others (Fig. 1(b)). The difference in the averaged wind vector between the two periods (2081 to 2100 and 1986 to 2005) is shown in Fig. 1(c) and (d) for the atmospheric layers of 1000 hPa (altitude of around 100 m) and 850 hPa (altitude between 1100 m and 2100 m), respectively. The main features of the lower layer are increase of north wind in southern China and increase of west wind in the high latitudes of the Pacific. In the higher layer, southwest wind increases in south east China and southwest coast of South Korea while west wind increases over high latitudes of the Pacific. The 850 hPa layer is of particular concern for long range transport of pollutants in the study area.

2.2. POPsLTEA

The domain of POPsLTEA covers the region of 25°N–50°N and 98°E–148°E as shown in Fig. 2, including eastern China, the Korean peninsula, and Japan. A small part of each of Mongolia and Russia is also within the domain. The environmental media modeled in POPsLTEA are air, soil, water (fresh water and sea water), sediment, and vegetation as individual compartments. Each of the air and the water compartments consists of two sub-compartments i.e., vapor and particulate matters in air and dissolved phase and suspended solids in surface water where chemical equilibrium was assumed between the two sub-compartments.

The multimedia structure of the individual model cells in POPsLTEA is schematically shown in Fig. S1. With homogeneous mixing assumption for chemicals in individual compartments of a given cell, POPsLTEA is mathematically a set of ordinary differential equations which can generally be expressed for the compartment i in the cell n as

$$\frac{d(V_iC_i)_n}{dt} = \left[\sum_{j=1}^{N_i} A_{ij}k^o{}_{ij}(C_{ij}{}^* - C_i) + \sum_{k=1}^{M_{ij}}\sum_{j=1}^{N_i} A_{ijk}(F_{ji}{}^k - F_{ij}{}^k)\right]x_n$$
$$+\left[\sum_{p=1}^{N_p} A_{np}\left(D^t{}_{np}(C_p - C_n)/\Delta x_{np} + (U_{pn}C_p - U_{np}C_n)\right)\right]_i + (R_{in} + S_{in})V_{in}$$

$(i \neq j, n \neq p)$

V_i: volume of the compartment i
C_i: concentration of a chemical of interest in i
N_i: total number of compartments exchanging the chemical with i