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Are the ratios of the two concentrations at steady state in the medium pairs of air-water, air-soil, water-soil, water-sediment, and soil-sediment?

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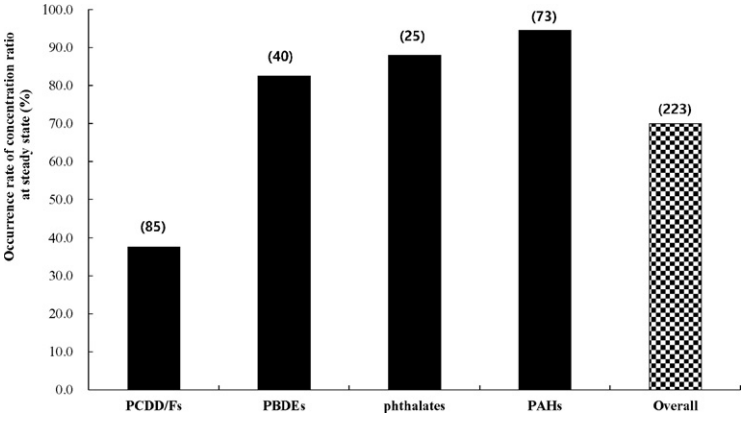
HIGHLIGHTS

- Use of concentration ratio for model optimization and evaluation
- Concentration ratios determined from concurrent multimedia monitoring data
- Identification of the concentration ratios that are at steady state
- Determination of the point values of the concentration ratios at steady state
- Implication of the steady state characteristics to model optimization and evaluation

GRAPHICAL ABSTRACT



The number in the parenthesis denotes the total number of temporal trends of the concentration ratio in each chemical group.

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ABSTRACT

For optimization and evaluation of a steady state multimedia model, concurrent multimedia monitoring data of steady state are necessary. In the lack of emission rate information, the primary aim of the present work was to assess if five concentration ratios (CRs) (C_{water}/C_{air}, C_{soil}/C_{air}, $C_{sediment}/C_{soil}$, C_{water}/C_{soil}, and $C_{sediment}/C_{water}$) of chemical compounds are at steady state in South Korea. A total of 16,676 CRs values were calculated using 74,641 concurrent multimedia (air, water, soil and sediment) monitoring data from 96 areas for 45 semi-volatile organic compounds (polychlorinated dibenzo-*p*-dioxins/furans, polybrominated diphenyl ethers, phthalates, and polycyclic aromatic hydrocarbons). Test of steady state indicated that CR is statistically at steady state with an overall occurrence rate of 70% of the 223 tested cases while the rates of individual chemical groups were 94.5%, 88%, 82.5%, and 37.6% for polycyclic aromatic hydrocarbons, phthalates, polybrominated diphenyl ethers, and polychlorinated dibenzo-*p*-dioxins/furans, respectively. About 83% of the steady state CRs resulted from scattering of two concentrations in each of the medium pairs without a certain temporal trend while the rest due to closely co-varying two concentrations. Analysis of the 95% confidence interval of the fugacity ratio indicated that CRs at steady state may occur in equilibrium state with higher chances than CRs at unsteady state. A total of 156 point values representing the CRs at steady state were determined that can be used for optimization

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and evaluation of steady state one-box multimedia models. However, potential influences of the uncertainties of the values arisen from the scattering of the concentration data should quantitatively be assessed in the model optimization and evaluation.

1. Introduction

The Act on Registration and Evaluation of Chemical Substances in South Korea requires submission of a chemical safety report where predicted environmental concentration at steady state is necessary for assessing the background environmental exposure at national scale for a chemical to be registered. Among existing multimedia models, SimpleBox (ECHA, 2012; van de Meent, 1995; van de Meent, 1993) has been recommended to use to calculate the predicted environmental concentration in South Korea (NIER, 2012a) as it has long been studied and widely used for screening-level exposure assessments (Armitage et al., 2007; Bakker et al., 2003; Berding, 2000; Berding and Matthies, 2002; Jager et al., 1998; Lijzen and Rikken, 2004; Palm et al., 2002; Struijs and Peijnenburg, 2002). Prior to the use, however, the model should be optimized in accordance with the environmental and meteorological conditions of South Korea and evaluated on its prediction performance.

Efforts to evaluate modified versions of SimpleBox for use in different regions have been made by comparing the predicted concentrations with the observed ones, but in limited manners. First, the comparisons were often made only on a single medium or two (Berding, 2000; Devillers et al., 1995; Kawamoto et al., 2001; Severinsen et al., 1996; Zhang et al., 2003) primarily due to the lack of multimedia monitoring data. Second, in a few studies where comparisons were presented for more than two media, the comparisons were conducted by using the data that were not produced from concurrent multimedia samplings (Gobas et al., 1998; Severinsen et al., 1996; Struijs and Peijnenburg, 2002; Zhang et al., 2003). Third, whether the observed concentrations were at steady state has not been assessed in previous evaluation studies except Lee et al. (2012). For the comparison, use of concentration data of steady state is appropriate as SimpleBox is a steady state model. Furthermore, poor model prediction was often ascribed to large uncertainties of the emission rate values (Kawamoto and Park, 2006; Lee et al., 2004; Palm et al., 2002), which also considerably limited the evaluation. The problem with the uncertain emission rate could be circumvented when the ratio of two concentrations for each of medium pairs (Jung et al., 2010; Lee et al., 2012; Lee et al., 2004; Song et al., 2014; Struijs and Peijnenburg, 2002; van de Meent, 1995) is used for the comparison. This is because the predicted concentration ratios (CRs) are independent of the emission rate in linear steady state multimedia models such as SimpleBox. These limitations strongly suggest that use of observed CRs (rather than concentration) at steady state that are determined from concurrent multimedia concentration data will lead to improved model evaluation.

As a preceding step to the optimization and evaluation of SimpleBox modified for use in South Korea, the main objective of the present work

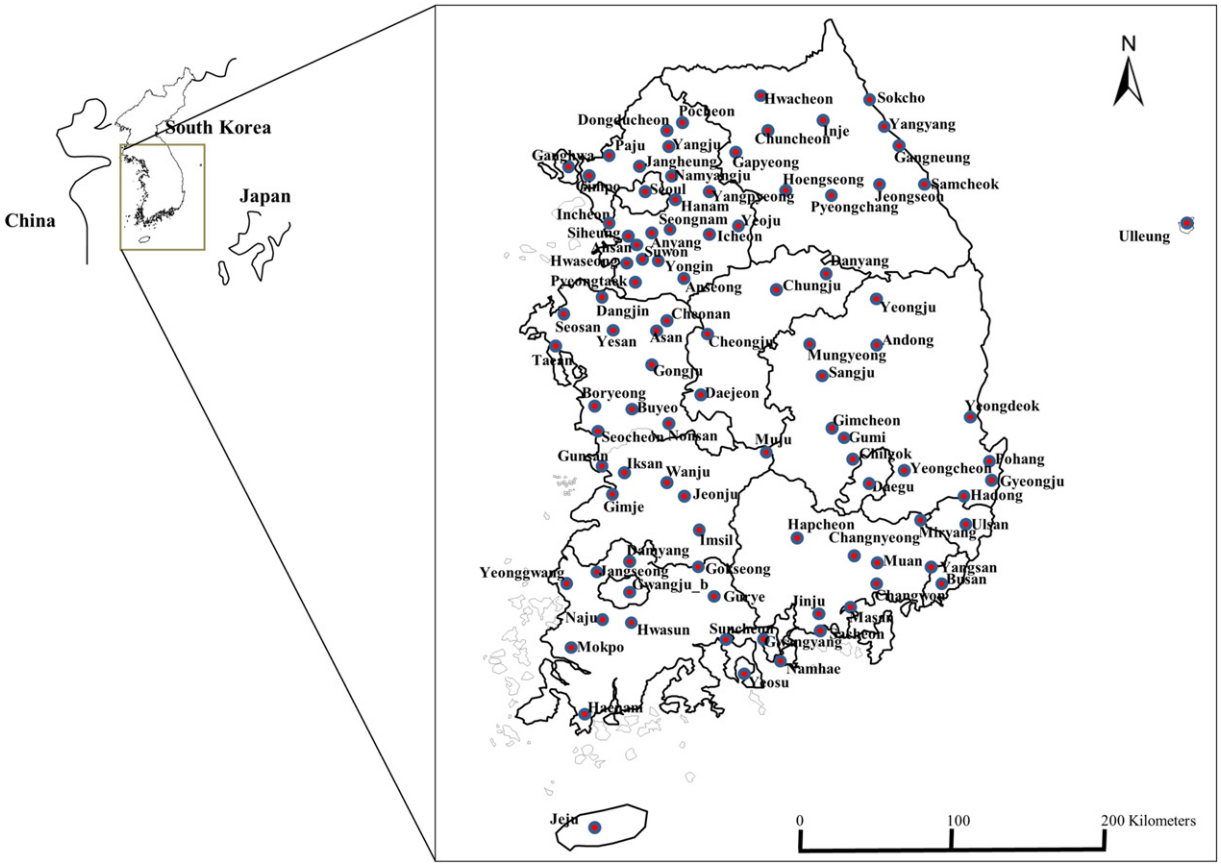

Fig. 1. Monitoring locations in the study area.