Evaluation of a multimedia fate model, POPsME for PAHs

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A dynamic multimedia model with 2-dimensional spatial resolution, POPsME (Persistent Organic Pollutants in Multimedia Environments), was evaluated by comparing predicted relative concentrations with those measured. A total of 12 polycyclic aromatic hydrocarbons (PAHs) were tested (phenanthrene, anthracene, fluoranthene, pyrene, chrysene, benz (a)anthracene, benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(a)pyrene, dibenz(a,h)anthracene, benzo(g,h,i)perylene, and indeno(1,2,3-c,d)pyrene). The concentrations were measured in air particulates, water (dissolved phase and suspended solids (ss)), soil, sediment, and leaves of *Pinus koraiensis* and *Prunus serrulata* at seven sites in the Seoul and neighboring area (150km x 150km), Korea.

POPsME is a mass balance model describing the changes in concentration in five well-mixed compartments-air, surface water, soil, sediment, and vegetation. Also sub-compartments are included in the compartments (e.g. particulate matters in air, suspended solids in water, and soil-air, soil-water, soil-solids in soil etc.). Vegetation is divided into 4 types (coniferous plant, deciduous plant, grass, and crops).

The use of the relative concentration, not the individual concentration in each medium, was proposed to evaluate the multimedia fate model. The relative concentration refers to the ratio of concentration in a medium to that in a reference medium, e.g., C_{air}/C_{soil} or C_{water}/C_{soil} if soil is chosen as a reference medium. The use of the relative concentration has certain advantages. First, the predicted relative concentration hardly changes with the total emission or emission rate if the emission ratios among multimedia are left unchanged. Therefore, uncertainties of emission estimates pose less problem for the model evaluation and the models can be improved without accurate emission estimates. Second, with an emphasis on the relative concentration, a model evaluation focuses on the model's capability to predict the relative concentrations among different media, i.e., the multimedia distribution, rather than the individual media concentration itself. Therefore, the relative concentration effectively serves for assessing chemical fate in the multimedia environment, which is a primary goal of the models. If a model is properly calibrated following this approach, an accurate prediction of the concentration in a medium would lead to accurate prediction of the ones in other media. Third, in dynamic models, the value of the predicted relative

concentration quickly stabilizes while individual concentrations are still transient. This condition substantially reduces the burden of choosing an appropriate simulation period to compare the model outcomes with measured data.

After the parameter adjustment to a degree that deviations of the predicted values fall within an order of magnitude from the measured ones (i.e. Phe, Pyr, BaP, and BghiP), POPsME was evaluated with the remaining eight PAHs (Ant, Fl, BaA, Chr, BbF, BkF, IcdP, and DahA).

Overall, the prediction and the observation agree with each other within approximately a factor of 10 for all PAHs in the multiple environmental media (e.g. C_{air}/C_{soil}, $C_{dissolved}/C_{soil}$, C_{ss}/C_{soil}, and $C_{sediment}/C_{soil}$). However, the model prediction tended to underestimate C_{ss}/C_{soil} and $C_{sediment}/C_{soil}$ for the PAHs of lower K_{ow} while overestimating for those of larger K_{ow}. This tendency is due to the increasing disparity between the measured partitioning equilibrium coefficient (K_{oc}) and the estimated one with K_{ow}.

In summary, a dynamic multimedia model, POPsME, was evaluated for a total of 12 PAHs. The evaluation was unique in that i) the model was tested in the absence of quantitative emission information by comparing the predicted relative concentrations with those measured, ii) the evaluation involved an extended number of environmental media (particulates in air, soil, dissolved phase, suspended solids, sediment, and vegetation), and iii) upon adjusting important parameters by using a set of measured data of four PAHs, the model prediction agrees with the observed multimedia distribution within one order of magnitude for the remaining eight PAHs. Taking into account the fact that the short-term data were used of which variability ranged from one to three orders of magnitude, it might not be appropriate to evaluate the performance of POPsME with accuracy that is less than the variability of the measured values.

The results demonstrate that multimedia models may effectively be evaluated by using the relative concentration while accurate emission estimates are not available. The use of the relative concentration, therefore, is proposed as a valuable means to evaluate and improve the model, particularly, for multimedia distribution of substances.