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A Multimedia Fugacity Model to Estimate the Fate and Transport of Polycyclic Aromatic Hydrocarbons (PAHs) in a Largely Urbanized Area, Shanghai, China

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Abstract Increasing PAHs pollutions is creating more complex urban pollution system. However, the availability of sufficient monitoring activities for PAHs in multicompartment and corresponding multi-interface migration processes is still not well understood. In this study, a Level III steady state fugacity model was validated to evaluate the detailed local variations, and mass fluxes of PAHs in various environmental compartments ($i.e.$, air, soil, sediment, water, vegetation and organic film). This model was applied to a region of Shanghai in 2012 based on a large number of measured data and brings model predictions in 2020. The model results indicate that most of the simulated concentrations agreed with the observed values within one order of magnitude with a tendency of underestimation for vegetation. Direct emission is the main input pathway of PAHs entering the atmosphere, whereas advection is the main outward flow from Shanghai. Organic film was achieved the highest concentration of PAHs compared to other compartments up to 58.17 g/m^3. The soil and sediment served as the greatest sinks of PAHs and have the longest retention time (2421.95-78642.09 h). Importantly, a decreasing trend of PAHs was observed in multimedia from 2012 to 2020 and the transfer flux from the air to vegetation to soil was the dominant pathways of BaP intermedia circulation processes. A sensitivity analysis showed that temperature was the most influential parameter, especially for Phe. A Monte Carlo simulation emphasized heavier PAHs were overpredicted in film and sediment, but lighter PAHs in air and water were generally underestimated.