Polymers as reference partitioning phase: polymer calibration for an analytically operational approach to quantify multimedia phase partitioning - DTU Orbit (08/11/2017)

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Polymers are increasingly applied for the enrichment of hydrophobic organic chemicals (HOCs) from various types of samples and media in many analytical partitioning-based measuring techniques. We propose using polymers as a reference partitioning phase and introduce polymer-polymer partitioning as the basis for a deeper insight into partitioning differences of HOCs between polymers, calibrating analytical methods, and consistency checking of existing and calculation of new partition coefficients. Polymer-polymer partition coefficients were determined for polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and organochlorine pesticides (OCPs) by equilibrating 13 silicones, including polydimethylsiloxane (PDMS) and low-density polyethylene (LDPE) in methanol-water solutions. Methanol as cosolvent ensured that all polymers reached equilibrium while its effect on the polymers' properties did not significantly affect silicone-silicone partition coefficients. However, we noticed minor cosolvent effects on determined polymer-polymer partition coefficients. Polymer-polymer partition coefficients near unity confirmed identical absorption capacities of several PDMS materials, whereas larger deviations from unity were indicated within the group of silicones and between silicones and LDPE. Uncertainty in polymer volume due to imprecise coating thickness or the presence of fillers was identified as the source of error for partition coefficients. New polymer-based (LDPE-lipid, PDMS-air) and multimedia partition coefficients (lipid-water, air-water) were calculated by applying the new concept of a polymer as reference partitioning phase and by using polymer-polymer partition coefficients as conversion factors. The present study encourages the use of polymer-polymer partition coefficients, recognizing that polymers can serve as a linking third phase for a quantitative understanding of equilibrium partitioning of HOCs between any two phases.

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