



Contents lists available at ScienceDirect

Marine Pollution Bulletin

journal homepage: www.elsevier.com/locate/marpolbul

Review

Review of the partitioning of chemicals into different plastics: Consequences for the risk assessment of marine plastic debris

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ARTICLE INFO

Article history:

Received 28 February 2016
 Received in revised form 15 July 2016
 Accepted 16 July 2016
 Available online xxxx

Keywords:

Plastic water partition coefficients
 Marine plastic debris
 Persistent organic pollutants
 Polyethylene

ABSTRACT

Marine plastic debris are found worldwide in oceans and coastal areas. They degrade only slowly and contain chemicals added during manufacture or absorbed from the seawater. Therefore, they can pose a long-lasting contaminant source and potentially transfer chemicals to marine organisms when ingested. In order to assess their risk, the contaminant concentration in the plastics needs to be estimated and differences understood. We collected from literature plastic water partition coefficients of various organic chemicals for seven plastic types: polydimethylsiloxane (PDMS), high-density, low-density and ultra-high molecular weight polyethylene (LDPE, HDPE, UHMWPE), polystyrene (PS), polypropylene (PP), and polyvinyl chloride (PVC). Most data was available for PDMS (1060) and LDPE (220), but much less for the remaining plastics (73). Where possible, regression models were developed and the partitioning was compared between the different plastic types. The partitioning of chemicals follows the order of $LDPE \approx HDPE \geq PP > PVC \approx PS$. Data describing the impact of weathering are urgently needed.

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Contents

1.	Introduction	0
2.	Methodology	0
2.1.	Data collection	0
2.2.	Data quality control and exclusion of data	0
2.3.	Data treatment and regression analysis	0
3.	Results and discussion	0
3.1.	Models for LDPE and PDMS	0
3.1.1.	LDPE	0
3.1.2.	PDMS	0
3.1.3.	Alternative descriptors: Abraham solvation parameters	0
3.1.4.	Regressions reported by other studies	0
3.2.	Partitioning into other plastic types: PP, PVC, PS, UHMWPE and HDPE	0
3.3.	Extrapolation to marine plastic debris: the role of ionic strength, temperature and weathering	0
3.3.1.	Ionic strength	0
3.3.2.	Temperature	0
3.3.3.	Weathering	0
3.4.	Uncertainties	0
3.5.	Mechanistic considerations	0
3.5.1.	LDPE and PDMS	0
3.5.2.	LDPE, HDPE and PP	0
3.5.3.	PVC and PS	0
3.6.	Implications for risk assessment of plastic debris	0

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Funding information	0
Appendix A. Supplementary data	0
References.	0

1. Introduction

There are wide concerns regarding plastic wastes being released into marine systems: A recent report estimated that 5.25 trillion particles are floating in the world's oceans (Eriksen et al., 2014). Marine plastic debris are ingested by marine species, leading to various adverse effects such as reduced food uptake or mechanic injuries. In addition, plastic debris contain chemicals, either because they were added during manufacturing with the aim of giving the plastic flexibility, durability and color, or because they were absorbed from the surrounding seawater like e.g. persistent organic pollutants (POP) (Mato et al., 2000; Rios et al., 2007; Teuten et al., 2009; Gauquie et al., 2015). Although preliminary studies indicated that the risk of contaminant transfer directly from plastic to the organism might be limited compared to other exposure routes (Besseling et al., 2012; Koelmans et al., 2013; Gouin et al., 2011; Herzke et al., 2015), the situation could be different for chemicals that are less abundant in the food chain (Tanaka et al., 2013). In addition, due to the low degradability of the plastic particles, they can potentially act as a long lasting source of chemicals, where weathering might also influence the sorption and release of chemicals.

Assessing the risk of contaminants absorbed by plastic debris requires the estimation of the actual concentration of the pollutants in the plastics, and the understanding how they vary between the different plastic types. The plastics most often found in oceans comprise low density and high density polyethylene (LDPE and HDPE), polypropylene (PP), polyvinylchloride (PVC) and polyethylene terephthalate (PET) (Rochman et al., 2012). So far, only few studies quantified or monitored the sorption of chemicals to plastic pellets or debris under field condition (e.g. Ref. Mato et al., 2000; Rochman et al., 2012; Endo et al., 2005), and even fewer related the observed concentrations directly to the average concentration in the seawater. Deriving partition coefficients from field monitoring data is difficult as usually the previous residence places of the plastic particles are unknown. However, partitioning into some plastic types has been intensively studied in laboratories, where e.g. polydimethylsiloxane (PDMS), and low density polyethylene (LDPE) are widely used in solid phase micro extraction (SPME). The properties of LDPE and PDMS have been reviewed by, e.g., DiFilippo and Eganhouse (2010) and Lohmann (2011). Limited amount of data are also available for other plastic types such as PP, PVC and PS.

The plastics considered in the present study are made of apolar polymers, and the partitioning of a chemical from the water into the plastic is mainly driven by hydrophobicity (Dean et al., 1996). A commonly used descriptor for hydrophobicity is the octanol-water partition coefficient K_{ow} , and most studies correlated the measured plastic-water partition coefficient $\log K_{pw}$ with the corresponding $\log K_{ow}$, e.g. Poerschmann et al. (2000), Smedes et al. (2009), Hsieh et al. (2011) or Atkinson and Duffull (1991) to name just a few. Other descriptors used in models for plastic-water partitioning include water solubility, heptane-water partition coefficient, or the Abraham salvation model (DiFilippo and Eganhouse, 2010; Lohmann, 2011).

The aim of our study was to compare the partitioning of various organic chemicals ($\log K_{ow}$ ranging from 0.90 to 8.76) between water and five types of plastic found in the environment: LDPE, HDPE, PP, PS and PVC. All studies found were performed in the lab, except two studies with PCB in PP (Mato et al., 2000), and PAH in HDPE and LDPE (Müller et al., 2001). We focused on apolar organic chemicals due to their high environmental importance and data availability but polar chemicals were included where available. For comparison, we also included data

on PDMS, a well-studied surrogate for sorption to organic matter. Covering a broad range in K_{ow} and K_{pw} increases the understanding of how chemicals partition into plastics. $\log K_{pw}$ was correlated to $\log K_{ow}$ for each chemical group and plastic type, evaluating differences between the plastics. K_{ow} was chosen as descriptor because it has been successfully used before, it is easy accessible and a single descriptor was favored to facilitate the comparison between the different plastics. Yet, links between $\log K_{pw}$ values and Abraham descriptors were explored as well. Subsequently, we discuss environmental factors, esp. temperature, ionic strength of seawater and weathering, relevant for extrapolation to marine plastic debris, and where possible, results are compared to the available field observations. Conclusions and outlook for future research needs are discussed to improve the risk assessment of marine plastic debris.

2. Methodology

2.1. Data collection

A literature review was conducted to collect plastic-water partitioning ratios for various PCB congeners and other chlorinated chemicals, polycyclic aromatic hydrocarbons (PAH), polybrominated diphenyl ethers (PBDE), alkanes, organophosphorous pesticides, and other organic chemicals (see Table 1 and Supporting Information). Only published, peer reviewed studies were examined. The studies measured the partitioning into polydimethylsiloxane (PDMS), low density- polyethylene (LDPE), polystyrene (PS), polypropylene (PP) and polyvinyl chloride (PVC). All studies found were performed in the lab, except two studies with PCB in PP² (field sorption experiment with pellets during 7 days), and PAH in HDPE and LDPE (Müller et al., 2001) (passive samplers in an estuarine during 32 days). Partition coefficients related to air such as air-PDMS were not included because 1) converting $K_{PDMS-air}$ to $K_{PDMS-water}$ would have added additional uncertainty, and 2) such data were considered less relevant regarding the ultimate aim of this study. The few ionizing chemicals in the data set were measured at a pH > 1.7 log units above or below the corresponding pK_a such that <2% of the chemical was ionized. Therefore, the reported K_{pw} always corresponds to the unionized chemical. The search yielded in total 1348 data points, which were subsequently analyzed regarding their quality (see below). Final adjusted values (FAV) for K_{ow} were taken from Schenker et al. (2005) (PCBs and selected organochlorines), Ma et al. (2009) (PAH) and Wania and Dugani (2003) (PBDEs). For congeners where no FAV data were available, we used the regressions with molecular weight as reported in the three studies to estimate the K_{ow} . Studies deriving FAV values referred either to “wet octanol”, i.e. octanol saturated with water like in the experimental K_{ow} set up, or to “dry octanol” as used e.g. in air-octanol experiments. The solubility properties of dry and wet octanol are different and a conversion is needed. In the present study, dry K_{ow} (K_{ow}^*) was converted to wet K_{ow} using the equation described in Schenker et al. (2005), i.e. $\log K_{ow} = (\log K_{ow}^* - 1.58) / 1.35$. If no FAV K_{ow} value were available, the K_{ow} values were taken from EpiSuite Kowwin v1.68, and measured values were preferred over estimated values.

2.2. Data quality control and exclusion of data

Large discrepancies regarding K_{pw} have been noted between laboratory studies using the classical experimental design where a clean plastic fiber was added into the water containing the pollutant of

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