Supplementary Material 1: Data quality and uncertainty analysis

In order to measure the data quality of data from the literature, the pedigree matrix approach, which was first introduced by Funtowicz and Ravetz (1990) and was adapted by Weidema and Wesnæs (1996) for life cycle inventory data, was adapted for this publication and applied to SSDR and redistribution rates. Additionally, the pedigree matrix approach used in the ecoinvent database for calculating life cycle inventory data uncertainty is also considered (Ciroth et al. 2016; Frischknecht et al. 2005; Muller et al. 2016; Wernet et al. 2016).

The data quality indicators were defined as follows:

- The reliability considers the quality of a data source and whether data generation such as sampling and analytical methods were documented, whether scientific methods were employed and whether the documentation was peer-reviewed. For reliability, even a good data quality (data quality indicator score (DQIS) = 1) implies uncertainty.
- Completeness considers two different aspects; in completeness 1, the comparability of the experiment conditions with real-world conditions, and in completeness 2, the degree of degradation measured at the end of the experiment. Since we aimed to assess the fate of an emission based on its half-life within the environment, the experiments that lasted long enough to measure the degradation of 50 percent or more did not add uncertainty to the completeness 2 indicator. Experiments that only lasted long enough to measure less than 50 percent degradation were assigned a score between 1 and 4. For completeness 1 and 2, a good data quality (DQIS = 1) does not evoke uncertainty.
- The temporal correlation considers the time difference between the year an experiment was conducted and today, based on the assumption that measurement and analytical methods might not have been as precise in the past as they are today. Nevertheless, we assume that this impact on the data quality is small. For the temporal correlation, a good data quality (DQIS = 1) does not add uncertainty.
- The geographical correlation refers to the congruence of an experiment location to our geographical reference; Germany. Since we saw considerable differences in data points depending on the humidity of the soil and the temperature of the water or the soil, the geographical correlation highly influences the overall uncertainty of a data set. For the geographical correlation, a good data quality (DQIS = 1) does not add uncertainty.
- The measurement method used assigns better scores when a combination of measurement methods was used and particularly low scores for experiments that relied on visual examination or crystallinity measurement. For the measurement method, even a good data quality (DQIS = 1) adds uncertainty.

The quality of expert judgments depends on the foundation of the judgment, e.g., whether the judgment is based on (an empirical) database, the experts' qualification, and the transparency of the procedure by which the judgment was obtained (Laner et al. 2016).

DQIS indicate good data quality (1) up to low data quality (4) (Kawecki and Nowack 2019). The data quality for each date was assessed based on the following Pedigree matrix:

Table 1 Pedigree matrix for degradation rates and transfer coefficients between environmental compartments (adapted from Weidema and Wesnæs 1996 and Laner et al. (2016))

		Score			
Indicator & Indicator Sensibility (a)	**Definition**	**1**	**2**	**3**	**4**
Reliability a = 0.75	Focus on the data source: documentation of data generation, e.g., assessment of sampling method, verification methods, reviewing processes.	The methodology of data generation is well documented and consistent, peer-reviewed data	The methodology of data generation is described but not fully transparent; no verification	The methodology of data generation is not comprehensively described, but the principle of data generation is clear; no verification	The methodology of data generation is unknown, no documentation available
Completeness 1 a = 1.5	Alignment of the degradation experiment to real-world conditions	Experiment under real-world conditions, e.g., degradation measurement took place in the environmental compartment, which is under investigation	Experiment with a real-world medium conducted in the lab under near-natural conditions	Lab experiment trying to reproduce real-world conditions, e.g., degradation measurement was done in the lab with an artificial medium, but pH value and temperature of the investigated environmental compartment was reproduced	Lab experiment without reproducing real-world conditions, e.g., artificially adding microorganisms to accelerate degradation or using temperature which is not observed in nature
Completeness 2 a = 1.5	Degree of degradation measured	The experiment lasted long enough to measure at least 50 % degradation	The experiment lasted long enough to measure at least 30 % degradation	The experiment lasted long enough to measure at least 10 % degradation	The experiment lasted long enough to measure less than 10 % degradation
Temporal correlation a = 0.375	Time difference to the year of study	Less than 5 years of difference to the year of study	Less than 10 years of difference to the year of study	Less than 15 years of difference to the year of study	Age of data unknown or more than 20 years of difference to the year of study
Geographical correlation a = 1.5	Congruence of the available date and the ideal date concerning geographical reference	Value relates to the studied region	Value relates to a region with similar conditions (climate zone and region (regarding the share of coasts, land, and rivers)	Value relates to very different conditions (climate zone and region regarding coasts, land, and rivers)	No explanation given regarding conditions (climate zone and region regarding coasts, land, and rivers) specified
Applied measurement method a = 1.5	Application of measurement method to investigate degradation rates	Combined measurement methods	One method of the following: CO_2 emission, biological oxygen demand	One method of the following: Area loss, Weight loss	One method of the following: Visual examination, Loss of crystallinity, Loss of viscosity

Expert judgment a = 2.5	Applied if the data was derived from an expert judgment	Formal expert elicitation with an (empirical) database; a transparent procedure and fully informed experts on the subject	Structured expert estimate with some empirical data available or using a transparent procedure with informed experts	Expert estimates with limited documentation and without empirical data available	An educated guess based on speculative or unverifiable assumptions

The a-values given in the first column of Table 1 indicate how the indicator's data quality influences the overall uncertainty of a data set. The DQIS of the input data sets can be found in Supplementary Material 2, in the sheets 'DQ of SSDR' and 'DQ of transfer coefficients'.

A coefficient of variation (CV) was calculated per input data set based on its DQIS according to equations (1) and (2) based on Laner et al. (2016) and Hedbrant and Sörme (2001). According to Laner (2016), the a and b values need to be defined by the modeler. In our case, the a-value differentiates between a non-sensitive case (a = 0.375), a medium sensitive case (a = 0.75), a highly sensitive case (a = 1.5), and an expert judgment case (a = 2.5), whereas the b-value is set to 1.105, as explained in Laner et al. (2016).

For data quality indicators reliability and measurement method, even a good data quality adds uncertainty according to equation (1).

$$\text{DQIS } [1, 4]\ CV = a \cdot e^{b \cdot score} \qquad \text{(Eq. 1)}$$

For uncertainty indicators completeness 1 and 2, temporal correlation, and geographic correlation, a good data quality does not add uncertainty according to equation (2).

$$\text{for DQIS } [1]\ CV = 0$$

$$\text{for DQIS } [2, 4]\ CV = a \cdot e^{b \cdot score - 1} \qquad \text{(Eq. 2)}$$

Table 2 indicates the CV for each indicator and score. For instance, Score 3 for the indicator reliability implies a CV of 20.6 %.

Table 2 CVs of the data quality indicators and scores

	Score			
Indicator	**1**	**2**	**3**	**4**
Reliabilty	2.3%	6.8%	20.6%	62.3%
Completeness1	0.0%	4.5%	13.7%	41.3%
Completeness2	0.0%	4.5%	13.7%	41.3%
Temporal correlation	0.0%	1.1%	3.4%	10.3%
Geographical correlation	0.0%	4.5%	13.7%	41.3%
Measuremente method	4.5%	13.7%	41.3%	124.6%
Expert judgement	7.5%	22.8%	68.8%	207.7%

The total uncertainty per data set is calculated following equation (3) based on Muller et al. (2016).

$$CV_{tot} = \sqrt{\begin{array}{l}(CV_{reliability}^2 + 1) * (CV_{completeness1}^2 + 1) * (CV_{completeness2}^2 + 1) * \\ (CV_{temp.corr.}^2 + 1) * (CV_{geogr.corr.}^2 + 1) * (CV_{measurement}^2 + 1) - 1\end{array}} \quad \text{(Eq. 3)}$$

A lognormal distribution describes natural phenomena and is described by only positive values (Limpert et al. 2001). This behavior is also likely for SSDRs and redistribution rates. Hence, it is assumed that data distribution is lognormal (Limpert et al. 2001), and we need to calculate the geometric standard deviation (GSD or σ_g) as the descriptor of the variability. The CV_{tot} and GSD connection is given in equation 4 based on Muller et al. (2016).

$$\sigma_g = e^{\sqrt{\ln(CV_{tot}^2+1)}} \quad \text{(Eq. 4)}$$

In cases where more than one SSDR per polymer and compartment was found in the literature, the data set with the lowest uncertainty score (meaning the lowest CV or GSD) was used for further calculations. In cases where more than one data set had the same lowest uncertainty score, the geometric mean of the SSDRs in question was used. Afterward, the half-life ($\tau_{1/2}$) is calculated using equation 7 of the main text.

The GSD of $\tau_{1/2}$ equals the GSD of the prior calculated SSDR's GSD, as it is assumed that the characteristic length and shape induce no further uncertainty. This is assumed as the characteristic length and shape are inherent descriptors of the environmental flow itself and the half-life is only specified for this specific length and shape.

To calculate the fate factors (FFs), the redistribution rates described in Table 1 of the main text and in Supplementary Material 2 in the sheet 'DQ of transfer coefficients' are used. All redistribution rates are based on expert judgments relying on structured expert estimates with some empirical data available or using a transparent procedure with informed experts (DQIS = 2). FFs are calculated by using a Monte Carlo simulation and 10 000 iterations applied to equation 1 of the main article. In each iteration, the redistribution factors are normalized to 100 % as they represent shares and a derivation of 100 % would not make sense. Each FF is then described by the geometric mean and geometric standard deviation retrieved from each distribution calculated with the Monte Carlo simulation. For more information on calculating the FFs, the Python script for the FFs' uncertainty calculation is given in Supplementary Material 4 for reproducibility and traceability reasons.

References

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