Supporting information

Elucidating the Variability in the Hexabromocyclododecane Diastereomer Profile in the Global Environment

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Table S1 Literature-reported measured concentrations of HBCDD diastereomers in air and soil samples across the world
Measurements are obtained from monitoring reports and peer-reviewed journal articles. Included are measurements with the sampling environment explicitly described in the original texts and a sampling size greater than 1.

Sampling site	Medium	Description	Sampling time	Sampling size	Diastereomer composition			α/γ ratio	Ref.
					α-HBCDD	β-HBCDD	γ-HBCDD		
Production and industrial sites									
Shanghai, CN	Air	Industrial sites	2006	7	29.7%	13.1%	51.0%	0.6	1
Guangdong, CN	Soil	Industrial sites	2006-2008	32	6%-37%	3%-10%	54%-91%	0.06-0.7	2
Laizhou Bay, CN	Soil	Production sites	2010	15	20.4%	12.3%	67.3%	0.3	3
Tianjin, CN	Soil	Industrial sites	2015	13	41%	11%	48%	0.8	4
Weifang, CN	Soil	Production sites	2015	19	17%	11%	72%	0.2	4
Remote background areas									
Ny-Ålesund, NO	Air	Remote sites	2007	15	25%	n.d.	75%	0.3	5
Birkenes, NO	Air	Remote sites	2007	14	47%	6%	47%	1.0	5
Greenland, DK	Air(1)	Remote sites	2012	13	16%-69%	7%-20%	16%-78%	0.2-4.4	6
Sleeping Bear Dunes, MI	Air	Remote sites	2014	27	39%	9%	52%	0.8	7
Sturgeon Point, MI	Air	Remote sites	2014	25	50%	9%	41%	1.2	7
Populated urban and rural areas									
Bloomington, IN	Air	Small university town	2003	3	32%-78%	6.1%-12%	9.7%-61%	0.52-8.0	8
Guangzhou, CN	Air	Urban and suburban areas	2004	32	59%-68%	11%-13%	21%-27%	2.2-3.6	9
Shanghai, CN	Air	Urban area	2006	18	48%-52%	13%-17%	28%-30%	1.6-1.8	1
Birmingham, UK	Air	Urban-suburban transect	2012-2013	8	34%-51%	18%-28%	24%-43%	0.8-2.3	10
Stockholm, SE	Soil	Urban area	2012	4	49%-72%	8%-13%	16%-42%	1.2-4.6	11
Stockholm, SE	Soil	Rural area	2012	4	5%-65%	6%-11%	32%-84%	0.05-1.9	11
Chicago, MI	Air	Urban area	2014	18	40%	11%	49%	0.81	7

Cleveland, OH	Air	Urban area	2014	22	27%	18%	54%	0.5	7
Cangzhou, CN	Soil	Area with professional use(2)	2015	12	74%	15%	11%	7.0	4
Waste disposal sites									
Qingyuan, CN	Soil	E-waste recycling sites	2006-2008	31	36%-36%	5%-9%	55%-59%	0.6-0.7	2
Guiyu, CN	Soil	E-waste recycling sites	2006-2008	27	56%	10%	33%	1.7	2

Notes:

CN = China; NO = Norway; DK = Denmark; MI = Michigan, United States; IN = Indiana, United States; UK = United Kingdom; SE = Sweden; OH = Ohio, United States

(1) Concentrations in particulate phase.

(2) Formulation and cutting of flame-retarded polystyrene plastics before use.

Table S2 Properties of HBCDD diastereomers

Property	Symbol	α-HBCDD	β-HBCDD	γ-HBCDD	Reference
Molecular weight (g mol^{-1})	*MW*	647.1	647.1	647.1	[12]
Air-water partition coefficient at 25°C (-)	log K_{AW}	-4.36	-4.76	-4.23	[12]
Octanol-air partition coefficient at 25°C (-)	log K_{OA}	9.96	10.5	10.4	[12]
Octanol-water partition coefficient at 25°C (-)	log K_{OW}	5.38	5.47	5.80	[12]
Internal energy of air-water phase transfer (kJ mol^{-1})	ΔU_{AW}	76.2	80.7	80.0	(1)
Internal energy of octanol-water phase transfer (kJ mol^{-1})	ΔU_{OW}	-20.0	-20.0	-20.0	(1)
Internal energy of octanol-air phase transfer (kJ mol^{-1})	ΔU_{OA}	-96.2	-100.7	-100.0	(1)
Degradation half-life in air (h)	HL_{air}	31.2	31.2	31.2	[12]
Degradation half-life in soil (h)	HL_{soil}	2040	2040	2040	[12]
Degradation half-life in sediment (h) (2)	HL_{sed}	840	840	840	[12]
Degradation half-life in water and WWTP (h) (2)	HL_{water}	2040	2040	2040	[12]
Degradation half-life in landfill and dump (h)	HL_{waste}	13032	13032	13032	[13]
Degradation half-life in vegetation (h)	HL_{veg}	2040	2040	2040	[12]
Activation energy for degradation in atmosphere (kJ mol^{-1})	E_{air}	10	10	10	(3)
Activation energy for degradation in soil (kJ mol^{-1})	E_{soil}	20	20	20	(3)
Activation energy for degradation in sediment (kJ mol^{-1})	E_{sed}	20	20	20	(3)
Activation energy for degradation in water and WWTP (kJ mol^{-1})	E_{water}	20	20	20	(3)
Activation energy for degradation in landfill and dump (kJ mol^{-1})	E_{waste}	20	20	20	-
Activation energy for degradation in vegetation (kJ mol^{-1})	E_{veg}	20	20	20	(3)

Note: (1) Calculated according to MacLeod et al.[14] based on Trouton's Rule and defaults.

(2) The same degradation half-lives are applied to the three diastereomers because earlier work observed no statistically significant difference in the kinetics of degradation of diastereomers in wastewater sludge and sediment.[15]

(3) Default values in BETR-Global 2.0.

Table S3 Global historical production of the technical HBCDD mixture as of 2015.

Region	Production period	Cumulative production (kilo tonnes)	Historical producing countries (number of producers)	Sources
RE1	2000-present (2015)	158.5 (26.6%)	China (>14[(1)])	16, 17
RE2	1985-2013	23.2 (3.9%)	Japan (>1)	18-22
RE3	1990-2006[(2)]	28.0 (4.7%)	Israel (1)	23, 24
			Turkey (unknown)	
RE4	2000-2004	1.1 (0.2%)	Russia (1)	24, 25
			Ukraine (1)	
			Czech (unknown)	
RE5	1965-present (2015)[(3)]	149.5 (25.1%)	Netherlands (1)	20, 21, 26, 27
			United Kingdom (1, before 2003)	
			Germany (1, before 1997)	
RE6	1965-present (2015)[(4)]	235.5 (39.5%)	United States (4)	26, 28, 29
RE7	Not available			

Notes:

(1) According to currently available information, there are at least 14 producers in China. However, the actual number is uncertain because of insufficient information. According to an announcement issued by China's Ministry of Environmental Protection on December 26, 2016, China is exempting production, use, import and export of HBCDD for manufacturing flame-retarded polystyrene insulation boards through December 25, 2021.*

(2) Back-calculated from the balance of global production and consumption.

(3) According to EU Commission Regulation 2016/293, production of HBCDD for manufacturing flame-retarded polystyrene insulation boards is allowed until November 26, 2019.†

(4) In the 2016 public Chemical Data Reporting (CDR), Albemarle and Chemtura reported production of HBCDD in the United States, with the tonnages claimed as "confidential business information (CBI)".[29] Production of HBCDD in the United States were reported to cease in 2016.[29]

* A Chinese version of the announcement is available at: http://www.mep.gov.cn/gkml/hbb/bgg/201612/t20161228_378327.htm

† Commission Regulation (EU) 2016/293 of 1 March 2016 amending Regulation (EC) No 850/2004 of the European Parliament and of the Council on persistent organic pollutants as regards Annex I. Available at: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=uriserv%3AOJ.L_.2016.055.01.0004.01.ENG

Table S4 Distribution of consumption of the technical HBCDD mixture among five applications

	AP1	AP2	AP3	AP4	AP5	Calculations
RE1	71.5%	26.5%	2.0%(1)	N.A.	N.A.	Taken from Li et al.[16]
RE2	8.5%	76.3%	15.2%	N.A.	N.A.	Calculated based on the lumped surveyed sales data between FR-polystyrene (84.8%) and FR-textiles (15.2%) for 2004-2011 in Japan.[18] Split between FR-EPS and FR-XPS based on the surveyed ratio of 1:9.[18]
RE3	50.0%	50.0%	N.A.	N.A.	N.A.	Assuming 50% of HBCDD each was used for FR-EPS and FR-XPS insulation boards due to a lack of information.
RE4	83.8%	16.2%	2.0%	6.0%	2.0%	Relative importance between AP1 and AP2 was calculated based on the relative market sizes of FR-EPS and FR-XPS between Western and Eastern Europe (30:17 and 10:1, respectively) and distribution ratio between AP1 and AP2 in RE5
RE5	43.0%	47.0%	2.0%	6.0%	2.0%	Taken from ESWI report,[30] which combined surveyed EU data for the years 2000[21] and 2006-2007[31]
RE6	43.0%	47.0%	<1%	7.0%	2.0%	Fraction used for textiles was collected from a USEPA report.[32] Because of a lack of available data, fraction for other applications were assumed to be same as those in RE5,[32] as indicated by Canada that "[t]he primary uses of HBCD in Canada (i.e., in EPS, XPS and textiles) are consistent with the ... global and European use patterns".[26]
RE7	50.0%	50.0%	N.A.	N.A.	N.A.	Assuming 50% of HBCDD each was used for EPS and XPS insulation boards due to a lack of information.

Note: (1) For the period 2000-2010.

Table S5 Net import and export fractions of the technical HBCDD mixture between regions.

Import fraction: Fraction of import to a region in the annual total international trade (import fractions to all regions sum up to 100%);
Export fraction: Fraction of export from a region in its annual total production.

Years	Import fraction[1]							Export fraction						
	RE1	RE2[2]	RE3[3]	RE4[4]	RE5	RE6	RE7[3]	RE1[5]	RE2	RE3	RE4	RE5[4]	RE6[6]	RE7
1990-1994		30%		70%								30%	25%	
1995-1999		30%		70%								20%	60%	
2000-2004		30%		55%			15%	37%				20%	70%	
2005-2009		30%	5%	50%			15%	37%				15%	70%	
2010-2014		25%	20%	40%			15%	37%				10%	70%	
After 2015		25%	20%	40%			15%						70%	

Notes:

(1) Due to a lack of information, we assumed no international trade of the technical HBCDD mixture for the years before 1990.

(2) Estimated based on the annual HBCDD consumptions of 600 – 2200 t for the period 1986 – 2001,[20] 555 – 1247 t for 2004-2011[18] in Japan, and the annual consumptions of 1500 t in 2011[33] and 1400~1600 in 2011-2014[34] in South Korea. Consumption data were rounded to nearest hundred and then extrapolated to fill gaps between reported years.

(3) Calculated based on the global mass balance. Due to a lack of information, we further assumed that the annual consumption in the rest of Asia (RE3) and the rest of the world (RE7) is proportional to their population defined in CiP-CAFE. Consumption data were rounded to nearest hundred and then extrapolated to fill gaps between reported years.

(4) Estimated based on the annual HBCDD consumptions in Europe, which were reported to be 8900 t in 1999,[20] 9500 t in 2001,[26] 9448 – 11186 t for 2003 – 2007,[35] 8913 and 9280 t in 2009 and 2010,[36] and 10000 – 125000 t in 2008 and 2011 – 2013.[37] We further assumed that the annual consumptions in Eastern (RE4) and Western Europe (RE5) are proportional to their population defined in CiP-CAFE. Consumption data were rounded to nearest hundred and then extrapolated to fill gaps between reported years.

(5) Taken from Li et al.[16]

(6) Estimated based on the historical records of annual HBCDD consumption of 3100 t for 1999,[20] 2800 t for 2001,[26] and 2200 – 2500 t for the period 2011-2015[34] in the United States, and the annual HBCDD consumption of 100 – 1000 t in Canada.[38] Consumption data were rounded to nearest hundred and then extrapolated to fill gaps between reported years.

Table S6 Emission and waste factors in CiP-CAFE modeling

Stage	Applications	Lower atmosphere	Wastewater		Soil
			Freshwater[1]	WWTP	
Production		4.0×10^{-5} [2]		1.2×10^{-7}	
Formulation	AP1	5.8×10^{-6}	6.3×10^{-5}	1.4×10^{-5}	
	AP2	7.3×10^{-6}	7.9×10^{-6}	6.6×10^{-5}	
	AP3	~0	~0	~0	
	AP4[3]	5.8×10^{-6}	6.3×10^{-5}	1.4×10^{-5}	
	AP5[4]	5.8×10^{-6}	6.3×10^{-5}	1.4×10^{-5}	
Processing	AP1	3.3×10^{-5}	1.4×10^{-6}	5.6×10^{-6}	
	AP2	1.7×10^{-5}	3.4×10^{-6}	1.4×10^{-5}	
	AP3	1.4×10^{-5}	1.8×10^{-3}	7.2×10^{-3}	
	AP4[3]	3.3×10^{-5}	1.4×10^{-6}	5.6×10^{-6}	
	AP5	3.0×10^{-7}	6.2×10^{-8}	2.4×10^{-7}	
Use	AP1	5.2×10^{-6}			
	AP2	6.9×10^{-6}			
	AP3	N.A.			
	AP4	N.A.			
	AP5	N.A.			
Service life	AP1	Calculated by EmissionRate[6]			
	AP2	Calculated by EmissionRate[6]			
	AP3[7]	1.27×10^{-4} (α-HBCDD); 1.44×10^{-4} (β-HBCDD); 1.46×10^{-4} (γ-HBCDD)			
	AP4	Calculated by EmissionRate[6]			
	AP5	Calculated by EmissionRate[6]			
Landfill		5.5×10^{-6}			6.0×10^{-5}
WWTP		Calculated by SimpleTreat			
Dumping		5.5×10^{-6}	1.1×10^{-4}		1.7×10^{-4}
Incineration		1.0×10^{-6}			
Recycling		9.0×10^{-6}			
Open burning[8]		0.612 (α-HBCDD); 0.205 (β-HBCDD); 0.056 (γ-HBCDD)			8.0×10^{-4} (α-HBCDD); 1.7×10^{-4} (β-HBCDD); 1.9×10^{-4} (γ-HBCDD)

Taken from Li et al.[16] unless indicated otherwise. (N.A. = Not applicable)

Notes:

(1) Taken from Li et al.[16], assuming that 80% of wastewater goes to WWTP and the rest is discharged into freshwater, in accordance with the EU Technical Guidance Document on Risk Assessment.[39]

(2) The average of atmospheric emission factors (ranging from 16 to 49 g t^{-1}; calculated by dividing the "total potential emissions" by the "total volume sold" in corresponding years) from member companies participating in the Voluntary Emissions Control Action Programme.[37]

(3) Since the EPS used in AP1 and AP4 are manufactured and processed in the same manner, we assume that emission factors in AP4 are identical to those in AP1.

(4) Assumed to be the same as emission factors in AP1, in accordance with the EU risk assessment report.[21]

(5) Here, "use" means (thermal) cutting of EPS and XPS insulation boards to fit the size of wall during installation.

(6) The following parameters are used for calculation on the EmissionRate model: Application model – open application; products in AP1 and AP2 are used outdoors (i.e., temperature-dependent), whereas products in AP4 and AP5 are used indoors (i.e., temperature-independent); materials in AP1 and AP4 are pervious, whereas materials in AP2 and AP5 are impervious. Partition coefficients between product material and gaseous phase ($K_{\text{product-gas}}$) are calculated using an empirical equation (suitable for "all materials") in Guo.[40]

(7) Calculated based on experimental data from Kajiwara et al.[41]

(8) Calculated based on experimental data from Ni et al.[42], in which waste polystyrene materials containing 5520 (α), 7120 (β) and 8150 (γ) ng $_{\text{HBCDD}}$ g^{-1}_{plastic} were subject to open burning, releasing 3380 (α), 1462.37 (β) and 458.67 (γ) ng $_{\text{HBCDD}}$ g^{-1}_{plastic} to air, and leaving 4.44 (α), 1.23 (β) and 1.57 (γ) ng $_{\text{HBCDD}}$ g^{-1}_{plastic} as residual ash (assumed to enter the soil). Unlike other tested plastics, polystyrene can be completely burned out, generating a substantial amount of airborne particles but no residual ash. The bulk of HBCDD in polystyrene transfers to and resides in the airborne particles, whereby it enters the atmosphere. Note that isomerization during open burning has been considered in the measurement.

Table S7 Fractions of polystyrene insulation boards (in AP1 and AP2) and packaging materials (in AP4) subject to recycling and reuse

	RE1	RE2	RE3	RE4	RE5	RE6	RE7
1965-1970							
1971-1980		0% (APs1&2)					
		1.0% (AP4)					
1981-1990		0% (APs1&2)					
		2.0% (AP4)					
1991-2000	0% (APs1&2)	0% (APs1&2)	0% (APs1&2)		9.8% (APs1&2)	0% (APs1&2)	0% (APs1&2)
	1.0% (AP4)	3.1% (AP4)	0.5% (AP4)		45% (AP4)	1.7% (AP4)	0.5% (AP4)
2001-2010	0% (APs1&2)	0% (APs1&2)	0% (APs1&2)		7.6% (APs1&2)	0.6% (APs1&2)	0% (APs1&2)
	1.0% (AP4)	4.8% (AP4)	0.9% (AP4)		55% (AP4)	12% (AP4)	0.2% (AP4)
2010-2015	0% (APs1&2)	0% (APs1&2)	0% (APs1&2)	0% (APs1&2)	7.6% (APs1&2)	0.6% (APs1&2)	0% (APs1&2)
	1.1% (AP4)	4.8% (AP4)	1.3% (AP4)	1.6% (AP4)	66% (AP4)	28% (AP4)	1.2% (AP4)
After 2016	9% (APs1&2)	0% (APs1&2)	0% (APs1&2)	0% (APs1&2)	7.6% (APs1&2)	0.6% (APs1&2)	0% (APs1&2)
	1.1% (AP4)	4.8% (AP4)	1.7% (AP4)	4.1% (AP4)	77% (AP4)	39% (AP4)	1.7% (AP4)

Source of historical data:

Data for RE1 are taken from Li et al.[16]

Record data of selected years for RE5 are taken from refs.[21, 43, 44] (for insulation boards) and refs.[43, 45] (for packaging materials). Extrapolated to the years without record data.

Record data of selected years for RE6 are taken from ref.[46] (for insulation boards) and ref.[47] (for packaging materials). Extrapolated to the years without record data.

For the rest regions, due to a lack of representative record data, we assume that insulation boards are neither recycled nor reused, whereas the recycling fractions of packaging materials are recycled in the same proportion as general solid waste.

Data for the period after 2016 are assumed to be the same as data in 2015.

Table S8 Isomerization factor matrixes

	IF (resulting in γ-dominant profile)	**IF** (resulting in α-dominant profile)
AP1[1]	$\begin{bmatrix} 1.00 & 0 & 0 \\ 0 & 1.00 & 0 \\ 0 & 0 & 1.00 \end{bmatrix}$	$\begin{bmatrix} 0.89 & 0 & 0.43 \\ 0.06 & 0.97 & 0.32 \\ 0.05 & 0.03 & 0.25 \end{bmatrix}$
AP2[2]	$\begin{bmatrix} 0.88 & 0 & 0.39 \\ 0.06 & 0.97 & 0.36 \\ 0.06 & 0.03 & 0.25 \end{bmatrix}$	
AP3[3]	$\begin{bmatrix} 0.90 & 0.18 & 0.18 \\ 0.04 & 0.78 & 0.10 \\ 0.06 & 0.04 & 0.72 \end{bmatrix}$	$\begin{bmatrix} 0.90 & 0.14 & 0.42 \\ 0.04 & 0.82 & 0.13 \\ 0.06 & 0.04 & 0.45 \end{bmatrix}$
AP4[1]	$\begin{bmatrix} 1.00 & 0 & 0 \\ 0 & 1.00 & 0 \\ 0 & 0 & 1.00 \end{bmatrix}$	$\begin{bmatrix} 0.89 & 0 & 0.43 \\ 0.06 & 0.97 & 0.32 \\ 0.05 & 0.03 & 0.25 \end{bmatrix}$
AP5[4]	$\begin{bmatrix} 0.90 & 0.19 & 0.80 \\ 0.04 & 0.77 & 0.11 \\ 0.06 & 0.04 & 0.09 \end{bmatrix}$	
Environment[5]	$\begin{bmatrix} 0.90 & 0.24 & 0.32 \\ 0.04 & 0.71 & 0.06 \\ 0.06 & 0.05 & 0.62 \end{bmatrix}$	

Algorithm to calculate IF:

According to eq.5 in the main text, we have

$$\begin{bmatrix} m_{\alpha,\text{after}} \\ m_{\beta,\text{after}} \\ m_{\gamma,\text{after}} \end{bmatrix} = \begin{bmatrix} \text{IF}_{\alpha\to\alpha} & \text{IF}_{\beta\to\alpha} & \text{IF}_{\gamma\to\alpha} \\ \text{IF}_{\alpha\to\beta} & \text{IF}_{\beta\to\beta} & \text{IF}_{\gamma\to\beta} \\ \text{IF}_{\alpha\to\gamma} & \text{IF}_{\beta\to\gamma} & \text{IF}_{\gamma\to\gamma} \end{bmatrix} \begin{bmatrix} m_{\alpha,\text{before}} \\ m_{\beta,\text{before}} \\ m_{\gamma,\text{before}} \end{bmatrix}$$

in which, $\left[m_{\alpha,\text{before}}, m_{\beta,\text{before}}, m_{\gamma,\text{before}}\right]^{\text{T}}$ describes diastereomer profile in products before thermal and light exposure, i.e., that measured in the technical HBCDD mixture,[48] and $\left[m_{\alpha,\text{after}}, m_{\beta,\text{after}}, m_{\gamma,\text{after}}\right]^{\text{T}}$

describes diastereomer profile after thermal and light exposure, i.e., that measured in end products in different applications (taken from literature-reported measurements).

Now define an error matrix:

$$\begin{bmatrix} \varepsilon_{\alpha,\text{after}} \\ \varepsilon_{\beta,\text{after}} \\ \varepsilon_{\gamma,\text{after}} \end{bmatrix} = \begin{bmatrix} m_{\alpha,\text{after}} \\ m_{\beta,\text{after}} \\ m_{\gamma,\text{after}} \end{bmatrix} - \begin{bmatrix} \text{IF}_{\alpha\to\alpha} & \text{IF}_{\beta\to\alpha} & \text{IF}_{\gamma\to\alpha} \\ \text{IF}_{\alpha\to\beta} & \text{IF}_{\beta\to\beta} & \text{IF}_{\gamma\to\beta} \\ \text{IF}_{\alpha\to\gamma} & \text{IF}_{\beta\to\gamma} & \text{IF}_{\gamma\to\gamma} \end{bmatrix} \begin{bmatrix} m_{\alpha,\text{before}} \\ m_{\beta,\text{before}} \\ m_{\gamma,\text{before}} \end{bmatrix}.$$

The best estimate of **iF** should minimize: $\varepsilon^2_{\alpha,\text{after}} + \varepsilon^2_{\beta,\text{after}} + \varepsilon^2_{\gamma,\text{after}}$,

$$\text{subject to: } \begin{cases} \text{IF}_{\alpha\to\alpha} + \text{IF}_{\alpha\to\beta} + \text{IF}_{\alpha\to\gamma} = 1 \\ \text{IF}_{\beta\to\alpha} + \text{IF}_{\beta\to\beta} + \text{IF}_{\beta\to\gamma} = 1 \\ \text{IF}_{\gamma\to\alpha} + \text{IF}_{\gamma\to\beta} + \text{IF}_{\gamma\to\gamma} = 1 \end{cases}.$$

Optimization of the above equations requires an initial value of **IF** (i.e., an *a prior* estimate). In this work, we choose the isomerization factor matrix describing photo-isomerization in the environment as the initial value because it can be directly calculated from experimental data in Harrad et al.[49] The Generalized Reduced Gradient (GRG) nonlinear solving method is used for optimization.

Notes:

(1) EPS is usually manufactured at low temperatures (80–120 °C). The diastereomer composition can remain the same as that in the technical HBCDD mixture (i.e., γ-dominant) or be altered slightly to a profile consisting of 46%(α) : 33%(β) : 21%(γ)[50] (i.e., α-dominant);

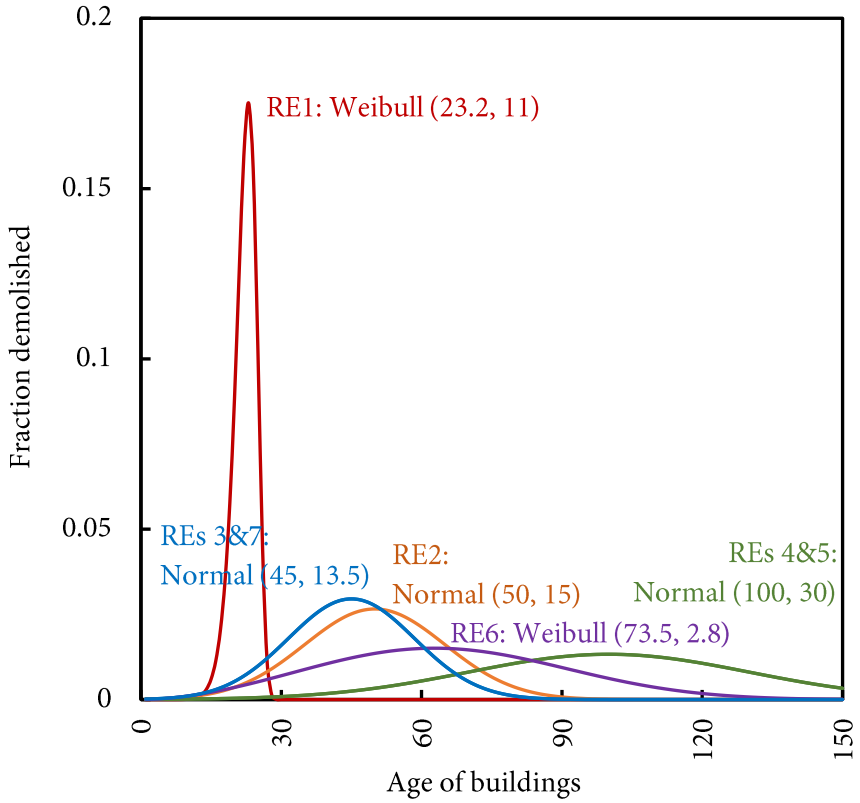
(2) XPS is usually manufactured at high temperatures (>120 °C). The diastereomer profile is already stable and thus unaltered when subject to further thermal processing;[50]

(3) HBCDD diastereomer profiles are rather diverse in different textile samples. Here we adopt two diastereomer profiles with the most abundant γ-HBCDD and α-HBCDD, respectively, from measurements in Kajiwara et al.[51];

(4) Given that HIPS is usually manufactured at very high temperatures (>180 °C), the diastereomer profile is assumed to be the same as that in equilibrium[52, 53] due to lack of measured data;

(5) Calculated based on experimental data in Harrad et al.[49]

Figure S1 Lifespan distribution of buildings in seven modeled regions



Note:

RE1: Lifespan distribution is taken from Cai et al.[54]

RE2: Based on Japanese data. Murakami et al.[55] compiled building lifespans in different parts of Japan, ranging from 38 (25th percentile) to 63 years (75th percentile). We assume that the average building lifespan in Japan is 50 years, and the standard deviation is 30% of the average.

RE3: Earlier studies assigned a lifespan of 40 years to Indonesian buildings,[56] and a lifespan of 50 years to Thai buildings.[57] We assume that the average lifespan is 45 years in RE3, and the standard deviation is 30% of the average.

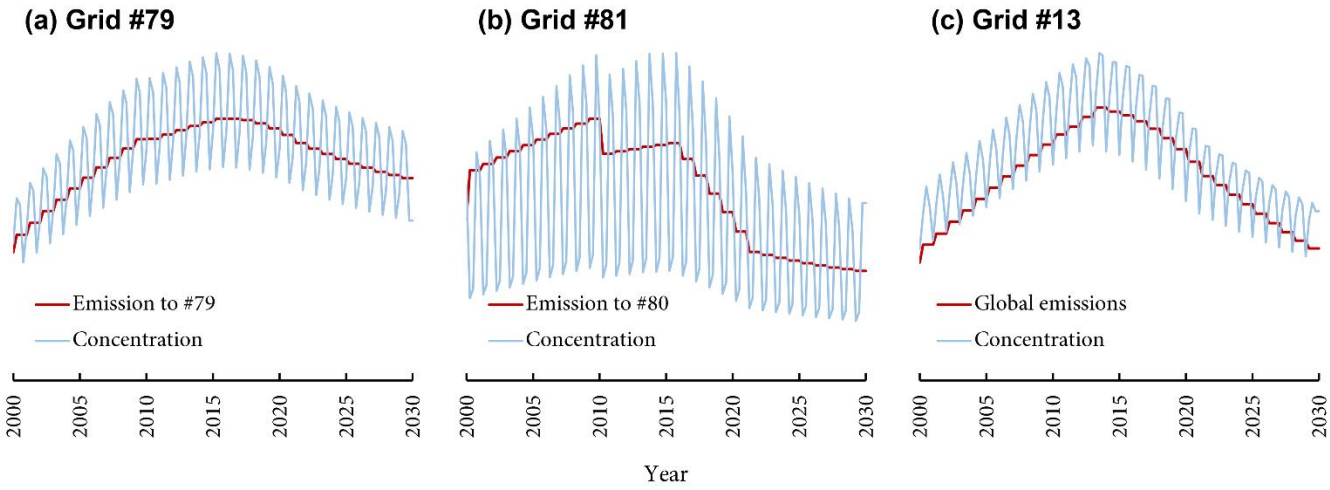
RE4: Lifespan distribution is assumed to be the same as that in RE5.

RE5: Earlier surveyed data demonstrate building lifespans of 68 – 80 years for Zurich, Switzerland (for the period 1970-2010)[58], 54 – 95 years for Spain[59], >180 years for Switzerland.[60] Earlier simulations assumed building lifespans of 100 years for the Netherlands,[61] and 60 (large and other buildings) – 90 (small buildings) years for Norway.[62] We assumed the average lifespan is 100 years for this region, and the standard deviation is 30% of the average.

RE6: Lifespan distribution is taken from Aktas et al.[63]

RE7: Lifespan distribution is assumed to be the same as that in RE3.

Figure S2 Response of modeled atmospheric concentrations in grid cells #79 (a), #81 (b) and #13 (c) to emissions



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