Environmental Fate and Transport Modeling for Perfluorooctanoic Acid Emitted from the Washington Works Facility in West Virginia

Supporting Information

Hyeong-Moo Shin[1], Verónica M. Vieira[2], P. Barry Ryan[3], Russell Detwiler[4], Brett Sanders[4], Kyle Steenland[3, 5], and Scott M. Bartell[6]

[1]School of Social Ecology, University of California, Irvine, CA
[2]Department of Environmental Health, Boston University, Boston, MA
[3]Department of Environmental Health, Emory University, Atlanta, GA
[4]Department of Civil and Environmental Engineering, University of California, Irvine, CA
[5] C8 Science Panel (http://www.c8sciencepanel.org)
[6]Program in Public Health, University of California, Irvine, CA

Table S1. Sources of data input and parameters

Model Component	Type of Input	Example parameter	Data Source	Time Scale
Air (ISCST3/AERMOD)	Emission sources	Annual emission rate, velocity	DuPont (2008)/Paustenbach (2007)	1951-2008
		Stack height, location		1951-2003
	Meteorological data	Mixing height	NOAA-NCDC	1951-2008
		Hourly wind direction, speed		
		Hourly precipitation rate		
	Particle information	Particle diameter, mass fraction, density	DuPont (2008)	1995/2004
	Building configuration	Building height, width, size	Paustenbach (2007)	1951-2003
	Receptor information	Terrain elevation	WebGIS	NA
Vadose Zone (PRZM3)	Source information	Deposition rate	AEMOD	1951-2008
	Precipitation	Hourly precipitation rate	NOAA-NCDC	
	Soil parameters	Soil type, hydrologic soil group	USDA-NRCS-STATSGO	NA
	Soil depth	Depth to groundwater table	DuPont (2003)/WebGIS	
	Chemical properties	Soil-water partition coefficient	Paustenbach (2007)	
Surface water (BreZo)	Emission sources	Annual liquid emission rate	DuPont/Paustenbach (2007)	1951-2008
	Bathymetric data	River bottom elevation	DuPont(2008)	NA
	River parameters	River width and depth	GIS	
	Mixing parameters	Flow velocity, mixing coefficient	Fisher (1979) /Akan (2006)	
		Monthly flow rate	USGS	1951-2008
Groundwater (MODFLOW-MT3D)	Source information	PFOA Flux to groundwater table	PRZM3/BREZO	1951-2008
	Base maps	River and drainage boundary	DuPont (2003)	NA
	Hydro-geological parameters	Hydraulic conductivity		
	Geological parameters	Recharge rate		
	Pumping well information	Historical pumping rate	Pipe network/DuPont (2003)	1951-2008

Table S2. Raw particle size distribution collected for the packed bed scrubber in the fine powder process areas of Washington Works under different conditions

| Particle size range (μm)	Mass fraction (%)			Particle size (μm)	Mass fraction (%)
	Condition 1	Condition 2	Condition 3		Condition 4
0-0.36	0.52	0.38	0.15	0-0.42	0.66
0.36-0.4	0.17	0.03	0.06	0.42-0.46	0.14
0.4-0.48	0.21	0.38	0.09	0.46-0.55	0.05
0.48-0.58	0.03	0	0.18	0.55-0.65	0
0.58-0.68	0.02	0	0.12	0.65-0.78	0.02
0.68-0.86	0.01	0	0	0.78-1.00	0.02
0.86-1.175	0.01	0.12	0.03	1.00-1.33	0
1.175-1.5	0.01	0.06	0.12	1.33-1.66	0
1.5-2.0	0	0.03	0.06	1.66-2.3	0.05
2.0-3.7	0	0	0	2.3-4.15	0.02
3.7-26	0	0	0.09	4.15-28.5	0.03
>26	0.01	0	0.09	>28.5	0.02
sum	0.99	1	0.99	sum	1.01

Table S3. Particle size distribution used in air dispersion modeling by Paustenbach et al. (2007) and Shin based on the particle size data in Table S2.

Paustenbach		Shin	
Particle size (μm)	Mass fraction (%)	Particle size (μm)	Mass fraction (%)
0.2	0.54	0.1	0.35
0.4	0.27	0.18	0.087
0.75	0.04	0.38	0.227
2.0	0.13	0.44	0.07
4.0	0.3	0.53	0.047
		0.63	0.003
		0.77	0.053
		1.0175	0.063
		1.3375	0.03
		1.75	0.00
		2.85	0.03
		14.85	0.033

Table S4. Observed: predicted water concentration ratio and calibration constant (φ) for each water district, for each of eight plausible values for log K_{oc}.

logK_{oc}	1.91	1.61	1.31	1.01	0.71	0.40	0.10	-0.20
Belpre	4.5	2.7	2.05	1.75	1.6	1.55	1.55	1.55
Little Hocking	2.85	2.55	2.3	2.15	2.1	2.05	2.05	2.05
Old Lubeck	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1
New Lubeck	1.9	1.85	1.75	1.7	1.7	1.65	1.7	1.75
Tuppers Plains	1.9	1.9	1.95	1.95	2	2	2.05	2.1
Mason County	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
Pomeroy	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
$\sum_{j=1}^{7}\left(\log\left(\varphi_j\right)\right)^2$	0.94	0.65	0.52	0.46	0.44	0.42	0.44	0.45

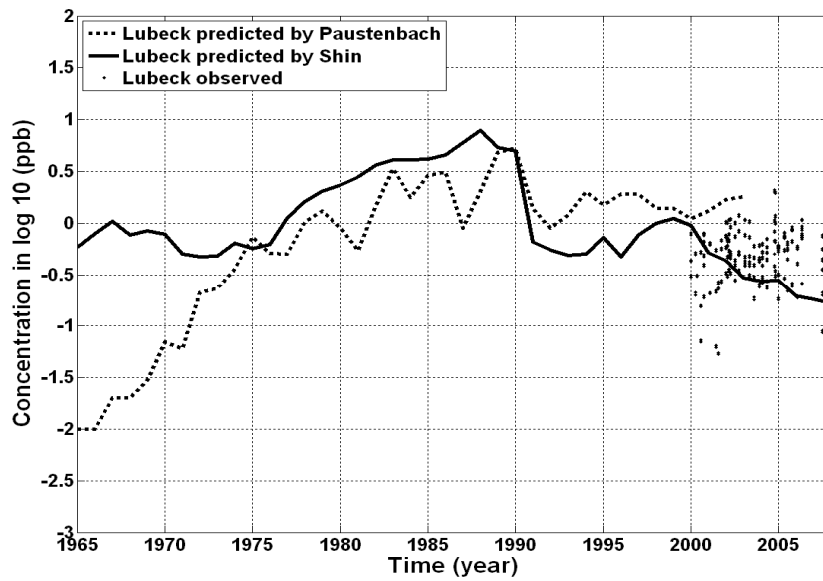**Figure S1.** Estimated historical PFOA releases into C8 Health Project study area
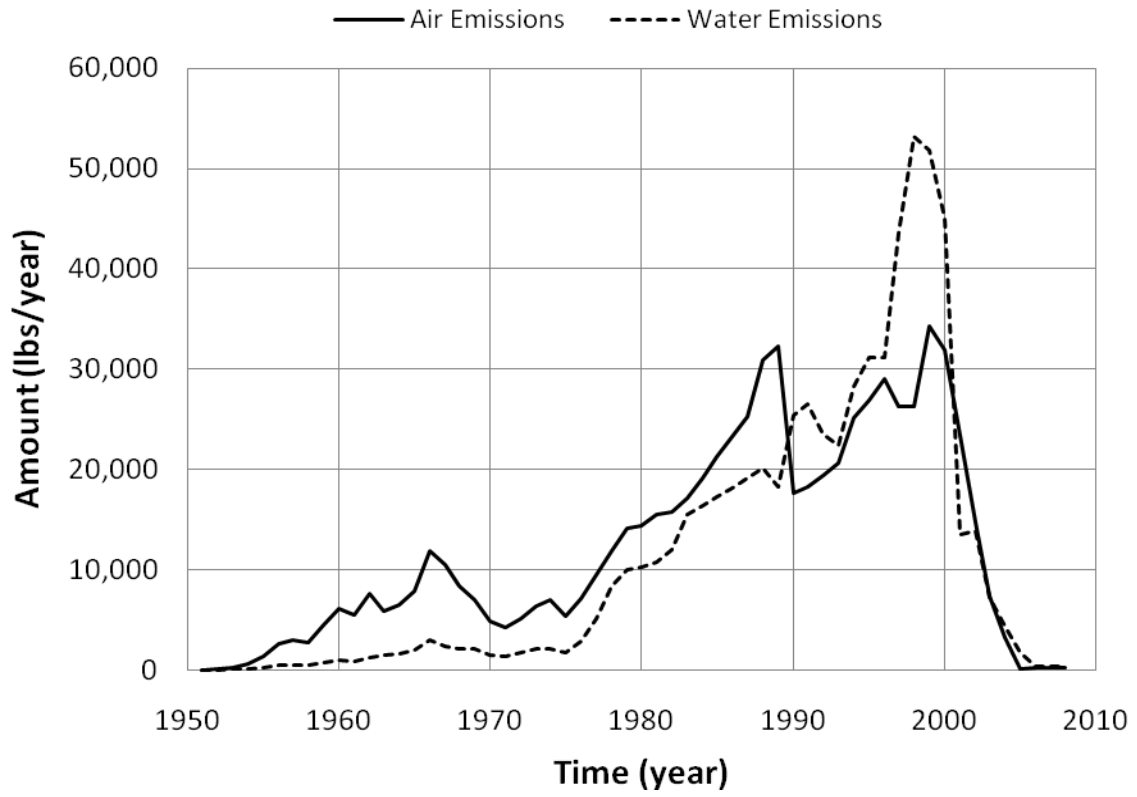
Figure S2. Observed (points) and annual average predicted calibrated log-10 concentration by Paustenbach (solid line) and Shin (dotted line). (a) Little Hocking well, (b) Lubeck well-predicted concentrations are combined with old (1960-1990) and new (1991-2008) Lubeck wells

(a)
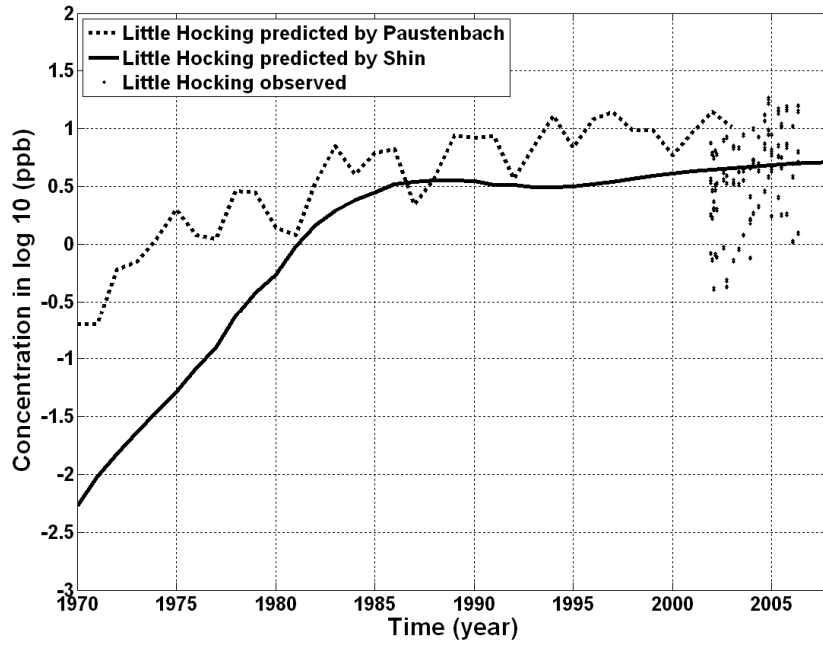
(b)

Scheme S1. Conceptual framework of fate and transport modeling