Estimating PFAS exposure across chemical, individual, and media using sparse published concentration summary statistics with the LEEM-R package

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Abstract

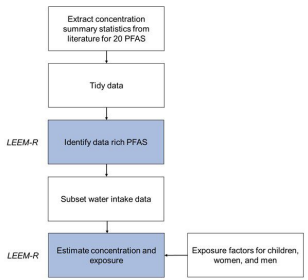
An established method for deterministic exposure estimates across media and chemicals is the product of pollutant concentration and a series of pathway-specific exposure factors. These estimates are strengthened with greater data resolution and more data sources, but results of chemical concentration in media are often published as summary statistics. To draw exposure estimates from sparse published summary statistics of concentration in media, the *Lorber-Egeghy-East Method R package* (LEEM-R) was developed.

- Concentration summary statistics for 20 PFAS were run using the model.
- LEEM-R returns lognormally distributed exposure estimates for any entered media.
- A drinking water exposure case example was performed for children, women, and children.
- The LEEM-R is available for pre-release and use for other exposure and concentration scenarios.

Methods

- Two inputs were required to run the model: summary statistics and exposure factors (Figure 1).
- To generate estimates representing many datasets, LEEM-R creates lognormal distributions from the geometric mean (GM) and geometric standard deviation (GSD).
- For this analysis, sample-size weighted GMs and GSDs are produced for each chemical and medium.
- Exposure estimates are generated by multiplying unique exposure factors across generated concentrations.

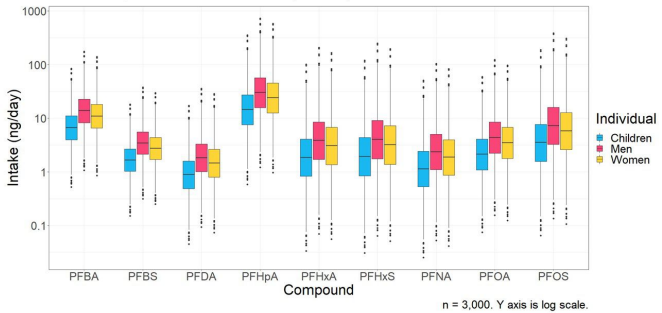
Figure 1.Generic Workflow for this application of the LEEM-R



- In 2021, PFAS concentration summary statistics were gathered across media (food, dust, water, products, blood, environment) for 20 different PFAS: PFOA, PFOS, PFNS, PFDS, PFHpA, PFDoA, PFUdA, PFPeA, PFHpS, PFPeS, 4:2 FTOH, 6:2 FTOH, 8:2 FTOH, 10:2 FTOH, PFBS, PFDA, PFHxA, PFHxS, PFNA, and PFBA.
- 1,080 total estimates are possible across 18 media, 20 PFAS and 3 different population groups (children, women, men).
- A case example for water intake was performed to demonstrate the LEEM-R using data from 'unimpacted' sites, with a sample size > 5, and excluding data from China.

Results

Figure 2. Water Intake Exposure Estimates for Adults, Women, and Children across PFAS



n = 3,000. Y axis is log scale.

- Results of the case example across sufficiently data-rich PFAS are depicted in Figure 3. PFHpA had the highest exposure estimate, at 30 ng/day, 24 ng/day and 3.2 ng/day for men, women, and children, respectively. Data are exclusively from studies in Europe and Brazil (Schwanz et al. 2016, Llorca et al. 2012, Domingo et al. 2012, Ericson et al. 2009).
- PFBA, PFOS, and PFOA are the next highest exposures, with intakes of 0.55, 0.16, and 0.12 ng/day across men, women, and children.
- 33/114 (37%) papers used for the drinking water estimates are from the United States.

Table 1. Counts of studies with sufficient summary statistics for use in LEEM-R across 20 PFAS in 'typical' scenarios

Media	10:2 FTOH	8:2 FTOH	6:2 FTOH	4:2 FTOH	**PFBA**	**PFBS**	**PFDA**	PFDoA	PFDS	**PFHpA**	PFHpS	**PFHxA**	**PFHxS**	**PFNA**	PFNS	**PFOA**	**PFOS**	PFPeA	PFPeS	PFUdA
Ambient Air	9	9	8	2	0	0	2	0	0	0	0	0	2	2	0	3	3	0	0	0
Biosolids	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	6	10	0	0	0
Consumer Products	2	2	2	1	4	3	4	1	1	1	1	3	2	4	1	5	4	1	1	1
Drinking Water	0	0	0	0	10	13	10	6	3	14	0	13	19	17	0	27	24	6	0	6
Food Packaging	9	9	8	0	0	0	1	2	0	12	0	1	1	1	0	1	1	0	0	0
Food (Breast Milk)	0	0	0	0	0	0	4	3	0	0	0	0	5	8	0	18	11	1	0	3
Food (Dairy)	0	0	0	0	1	0	1	0	0	1	0	0	0	1	0	5	5	0	0	0
Food (Fruit)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
Food (Meat)	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	7	19	0	0	0
Food (Other)	0	0	0	0	5	7	14	0	0	2	0	7	5	11	0	14	19	1	0	0
Food (Seafood)	0	0	0	0	0	0	0	5	14	10	6	1	1	0	0	12	27	18	0	14
Food (Vegetables)	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	4	0	0	0
Human blood*	0	0	0	0	1	3	31	0	0	0	1	1	40	35	0	41	43	0	0	3
Indoor Air	23	25	17	1	0	4	15	11	0	15	0	15	2	19	0	21	5	0	0	15
Indoor Dust	4	6	3	0	10	13	17	6	3	6	3	17	16	19	1	28	27	3	1	4
Landfill Leachate	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	1	1	0	0	0
Sediment	0	0	0	0	1	3	4	0	0	0	0	3	2	3	0	13	16	0	0	0
Sewage	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0	2	4	0	0	0
Soil	0	0	0	0	3	0	0	0	0	0	0	2	4	0	0	36	52	1	0	0
Wastewater Effluent	0	0	0	0	5	1	8	0	0	0	0	8	4	5	0	10	9	2	0	1
Wastewater Influent	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	2	2	0	0	0

*could be in plasma, serum, or cord. **no "human urine" typical data.

- Counts for usable datasets across all media in uncontaminated scenarios are listed in Table 1 above. PFAS selected in the water case example are in bold.
- Focus has largely centered on water, dust, and serum (blood), and PFOA, and PFOS. Air concentrations are rich for fluorotelomers (FTOHs).
- Aggregate exposure estimates across media is not possible for most PFAS given the current data landscape.

Discussion

Exposure Factors

- Exposure estimates for water intake were generated using assumptions of an absorption factor of 0.9 and intakes of 1.67 L/day, 2.75 L/day, and 3.46 L/day respectively for children, women, and men (EFH, NHANES). Daily 'Intake' estimates include drinking water, water in drinks, and water content in food.

*concentration (ng/L) = intake (L/day) * absorption factor*

- The LEEM-R can accept any number of exposure factors across populations. The importance of this function increases when two or more media are assessed, such as dust and water. A population subgroup with a high dust and water intake at a lower bodyweight will have a different exposure profile than one with low intakes and a higher bodyweight.

Aggregate Exposure and NHANES Validation

- Earlier versions of the LEEM-R have been used to estimate aggregate (total) exposure to PFOA and PFOS (Lorber & Egeghy, 2011, Egeghy & Lorber, 2011, East et al. 2021) by summing median exposure estimates from dietary intake, water ingestion, dust inhalation and dermal absorption, and indoor and outdoor air inhalation.
- Of the 20 PFAS, National Health and Nutritional Examination Survey (NHANES) data is available for 6 PFAS: PFDA, PFHxS, PFNA, PFOA, PFOS, and PFDoA (CDC, 2021). A Pharmacokinetic model can convert the daily intake to serum concentration for result validation. Without NHANES, serum concentrations are collected in this effort for validation (Table 1).
- Aggregate exposure estimates are only possible for data with sufficient data. Given the poor data paucity of food, reasonable estimates are only possible for PFOA and PFOS, though breast milk estimates for infants is available for PFOA, PFOS, PFDA, PFHxS, and PFNA.

The LEEM-R

Future Work

Evaluation of the 20 PFAS dataset and exposure estimates is ongoing. Results vary across data input (geography, impacted sites, collection methods, study quality), exposure factors, number of generated concentration points, and the weight prescribed to each study. Characterization of the inputs to the LEEM-R is the next step to producing reliable average media and exposure estimates for PFAS.

Model Development

The latest version of the LEEM-R Model, coded in R, is available with documentation at https://github.com/AlexanderEast/LEEMR or by running the following in R:

```
library(devtools)
install_github("AlexanderEast/LEEMR",force = TRUE)
library(LEEMR)
```

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