SUPPLEMENTAL FILE E: SHEDS-HT MODELING

Per- and Polyfluoroalkyl Substances (PFAS) Next Steps for Hazard, Exposure, and Risk Analyses
(CPSC Contract Number 61320622A0005, CPSC Order Number 61320623F2025)
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1. Inputs

1.1. Input Files

The default input files were downloaded from SHEDSHTRPackage/Inputs at master · HumanExposure/SHEDSHTRPackage · GitHub and used as-is with the exception of the following four input files. The revised versions used are included as attachments to this file:

- Attachment E-01_chem_props_pfas.csv = chemical properties file
- Attachment E-02_source_chem_pfas.csv = source chemicals file
- Attachment E-03_source_vars_pfas.csv = source variables file
- Attachment E-04_source_scen_pfas.csv = source scenarios file

Note that the attachments are .csv files and do not have a ReadMe tab as they are meant to be used as-is with SHEDS-HT.

1.2. Estimating y_0

The source chemicals file contains the y_0 parameter for articles, which is used in SHEDS-HT for estimating exposure to articles. y_0 is a measure of the gas-phase chemical concentration in the boundary layer of air next to the surface of the article. It assumes this concentration is in equilibrium. The two processes that affect the concentration are the ongoing emission of chemical from the article into the air, and the diffusion of chemical from the boundary layer into the general house air. As a practical matter, y_0 is measured in the absence of two effects: the ability of particles in the air to hold the chemical (which is not included because it depends on the number and size of the particles, which may vary), and the back-diffusion of chemical from the house air to the boundary layer. The SHEDS-HT code adjusts for the airborne particles. Chemical backflow is not relevant because SHEDS-HT is apportioning exposure to sources, and chemical from products or background sources is separate from the chemical originating in the article.

There are multiple ways to estimate y_0 theoretically. One is the dynamic approach of estimating a chemical emission rate from the article and the chemical diffusion (or convective mixing) rate from the boundary layer into the rest of the room. One problem is that little or no emission rate data is available in our data sources.

Another approach is to use fugacity calculations, as in the SHEDS-Fugacity model. Here, the fugacity (which is the chemical holding capacity) is derived from chemical properties and the physical properties of air and the article in question. Assuming equal fugacity for the article and the boundary layer air, the air/article chemical concentration ratio equals the fugacity ratio, based on the fugacity equation:

$$M = F * Z * V$$

Where:

M = mass (mol)
F = fugacity (Pa)
Z = fugacity capacity (mol/m^3/Pa)
V = volume (m^3)

Taking the volume to the other side, and converting mass from moles to grams using the molecular weight, MW, gives:

$$C = \frac{M * MW}{V} = F * Z * MW$$

Where:

C = concentration (g/m^3)
M = mass (mol)
MW = molecular weight (g/mol)
V = volume (m^3)
F = fugacity (Pa)
Z = fugacity capacity (mol/m^3/Pa)

This equation applies to both air and to the article. The fugacity capacities are given in Bennett and Furtaw, Jr. (2004).

For air:

$$C\_air = F\_air * Z\_air * MW$$

For the article:

$$C\_article = F\_article * Z\_article * MW$$

Hence, the concentration ratio when F_air = $F\_article$ is:

$$\frac{C\_air}{C\_article} = \frac{Z\_air}{Z\_article}$$

For vinyl flooring, from equation (18) in Bennett and Furtaw, Jr. (2004), the ratio $K_{va} = \frac{Z\_vinyl}{Z\_air}$ is given by:

$$K_{va} = \frac{1.58 * 10^5}{VP^{0.68}}$$

Where:

K_{va} = vinyl-air partition coefficient (-)
VP = vapor pressure (Pa)

For carpet, the expression for $K_{ca} = \frac{Z\_carpet}{Z\_air}$ from equation (20) in Bennett and Furtaw, Jr. (2004) is:

$$K_{ca} = \frac{6.60 * 10^3}{VP^{0.62}}$$

Where:

K_{ca} = carpet-air partition coefficient (-)
VP = vapor pressure (Pa)

Hence, for hard floors (vinyl or wood), if the concentration in the flooring is C_0, then the concentration y_0 in the boundary air layer is:

$$y_0 = C\_air = \frac{C_0}{K_{va}} = \frac{C_0 * VP^{0.68}}{1.58 * 10^5}$$

For carpet or for other textiles (sofa, etc.), the formula is:

$$y_0 = C\_air = \frac{C_0}{K_{ca}} = \frac{C_0 * VP^{0.62}}{6.60 * 10^3}$$

The y_0 for textiles is substantially larger than for hard, smooth surfaces, likely due to the presence of carpet bristles which increase the effective article-air surface area. While Bennett and Furtaw, Jr. (2004) do not discuss other textiles, which typically have fewer or no bristles, the above equation can be used for y_0, although this may result in an overestimate.

The above analysis assumes that C_0 and C_air (or y_0) are in the same units (as mass/volume). However, typically, concentration for solid materials is expressed in (ng/g), while C_air is not. In the SHEDS-HT code, y_0 is in (μg/m3).

If the concentration C is in (μg/g) and the density of the surface material is ρ (g/cm^3), then:

$$C_0 = C * \rho * 10^6$$

Where:

C_0 = concentration (μg/m^3)
C = concentration (μg/g)
ρ = density (g/cm^3)
10^6 = (cm^3/m^3)

Hence, for vinyl or hard floors:

$$y_0 = 6.3 * C * \rho * \mathrm{VP}^{0.68}$$

For carpet or textiles:

$$y_0 = 151 * C * \rho * \mathrm{VP}^{0.62}$$

Here, y_0 is in the SHEDS-HT units of (μg/m^3) while C is in (μg/g), ρ is in (g/cm^3) and VP is in Pa. For hard floors, assume ρ = 1.5 g/cm^3, while for carpet the value should be lower, p erhaps 1.0 g/cm^3.

1.3. Consumer Product–PUC Crosswalk

Because SHEDS-HT models exposure to product use categories (PUCs), individual consumer products from Holder et al. (2023) and Dewapriya et al. (2023) were first matched to a PUC based on the crosswalk shown in Table 1.

Table 1. Crosswalk of Individual Consumer Products to Product Use Categories.

PUC	PUC Description	Individual Consumer Products[a]
A.BM.CTG	Coatings	Coating
A.BM.CTG	Coatings	Paint
A.BM.CTG	Coatings	Stain
A.BM.CTG	Coatings	Water resisting paint
A.ET.LET	Large electronics	Screen
A.ET.LET	Large electronics	TV
A.ET.LET	Large electronics	Vacuum cleaner
A.ET.SET	Small electronics	Coffee maker
A.ET.SET	Small electronics	DVD cover
A.ET.SET	Small electronics	Keyboard
A.ET.SET	Small electronics	Mixed waste - small electronical devices
A.ET.SET	Small electronics	Switch
A.TX.BDD	Bedding	Bed cover
A.TX.BDD	Bedding	Bedding mattress protector
A.TX.BDD	Bedding	Bedding pillow protector
A.TX.BDD	Bedding	Blanket
A.TX.BDD	Bedding	Pillow fill
A.TX.CAR	Car textiles	Hyundai textile material
A.TX.CAR	Car textiles	Public transport seat cover
A.TX.CAR	Car textiles	Skoda textile material
A.TX.CPT	Carpet	Carpet
A.TX.CPT	Carpet	Carpet sample
A.TX.CPT	Carpet	Carpets/mats
A.TX.CPT	Carpet	Furnishings rugs
A.TX.CPT	Carpet	Persian carpet

PUC	PUC Description	Individual Consumer Products[a]
A.TX.CPT	Carpet	Pre-treated carpet
A.TX.CRT	Curtains	Curtain
A.TX.FRN	Furniture foam/textiles	Foam
A.TX.FRN	Furniture foam/textiles	Furnishings upholstery
A.TX.FRN	Furniture foam/textiles	Furniture polyurethane foam
A.TX.FRN	Furniture foam/textiles	Furniture seat cover
A.TX.FRN	Furniture foam/textiles	Furniture textiles
A.TX.FRN	Furniture foam/textiles	Tablecloth
A.TX.FRN	Furniture foam/textiles	Treated home textile and upholstery
A.TX.FRN	Furniture foam/textiles	Upholstery
A.TX.FRN	Furniture foam/textiles	Upholstery material
A.TX.INC	Inner clothing	Apparel kid's clothing
A.TX.INC	Inner clothing	Children's school uniforms
A.TX.INC	Inner clothing	Child's swimsuit
A.TX.INC	Inner clothing	Child's vest
A.TX.INC	Inner clothing	Infant clothes
A.TX.INC	Inner clothing	Treated apparel
A.TX.INC	Inner clothing	White t-shirt
A.TX.ODC	Outdoor clothing	Adult jacket
A.TX.ODC	Outdoor clothing	Children's weather-resistant outdoor wear (rainsuits, snowsuits, snowshoes, mittens)
A.TX.ODC	Outdoor clothing	Cotton/leather clothes
A.TX.ODC	Outdoor clothing	Gloves
A.TX.ODC	Outdoor clothing	Membranes for apparel
A.TX.ODC	Outdoor clothing	Outdoor jackets
A.TX.ODC	Outdoor clothing	Water repellant textiles
A.TX.TXT	Textile toy	Teddy bear cover
A.TX.TXT	Textile toy	Teddy bear filling
A.TX.VYF	Vinyl flooring	Laminated plastic floor covering
A.TX.VYF	Vinyl flooring	PTFE linoleum
P.AP.110.999	Body wax (car)	Car polish

PUC	PUC Description	Individual Consumer Products[a]
P.AP.110.999	Body wax (car)	Car wax
P.AP.110.999	Body wax (car)	Car wheel cleaner
P.AP.110.999	Body wax (car)	Lubricant for bicycles
P.AP.110.999	Body wax (car)	Tire shine
P.AP.140.000	Motor oil	Automotive lubricant oils
P.HM.020.000	Caulk or sealant	Sealant
P.HM.090.999	Lubricant	Lubricant
P.HM.090.999	Lubricant	Oil
P.HM.110.999	Multipurpose adhesive	Thread seal tapes and pastes
P.HM.110.999	Multipurpose adhesive	Thread sealant tapes and pastes
P.HM.110.999	Multipurpose adhesive	Thread sealing tape
P.HM.120.009	Paint (interior)	Coating
P.HM.120.009	Paint (interior)	Paint
P.HM.120.009	Paint (interior)	Stain
P.HM.120.009	Paint (interior)	Water resisting paint
P.IH.030.999	Automatic dishwashing detergent	Dishwashing liquid
P.IH.070.999	Carpet cleaner	Carpet care liquid
P.IH.070.999	Carpet cleaner	Carpet/fabric care liquids and foams
P.IH.070.999	Carpet cleaner	Commercial carpet-care liquids
P.IH.070.999	Carpet cleaner	Household carpet/fabric-care liquids and foams
P.IH.200.000	Floor polish	Floor polish
P.IH.200.000	Floor polish	Floor wax
P.IH.200.000	Floor polish	Floor waxes and stone/tile/wood sealants
P.IH.200.000	Floor polish	Treated floor waxes and stone/wood sealants
P.IH.330.000	Shoe polish or protectant	Shoe polish
P.IH.SKI	Ski polish	Ski wax
P.LY.010.005	Cleaner (exterior)	Deck cleaner

PUC = product use category.
[a]Individual consumer products were obtained from Holder et al. (2023) and Dewapriya et al. (2023). Specific sample numbers were removed (e.g., curtain 2) so that only the generic name is shown in the table.

2. Outputs

Separate model runs were performed for (i) products and (ii) articles. Each run produces the following outputs:

- [CASRN]_all.csv = modeled output for the 100,000 simulated individuals (i.e., each row is a simulated individual)
- [CASRN]_all_srcMeans.csv = mean value across the population for various exposure variables by PUC
- [CASRN]_allstats.csv = statistics (e.g., mean, standard deviation) calculated on the simulated individuals for multiple exposure metrics

Only the first two output files were used (see next paragraph). For convenience, the product and article outputs were consolidated into one file for each chemical and included as attachments to this file (Attachments E-05 to E-13).

Because we are interested in exposure metrics for the subpopulation of simulated individuals with non-zero product exposures, specifically for individuals that use at least one product (i.e., users of at least one article but no products were not included), only the [CASRN]_all.csv file for products was postprocessed to determine population statistics (e.g., mean, standard deviation). For chemicals that did not have any product PUCs, the [CASRN]_all.csv file for articles was used. The resulting statistics were used, along with the [CASRN]_all_srcMeans.csv file, to estimate the % contribution of each PUC to total exposure. The two postprocessed outputs were consolidated into one output file with the tabs shown below and included as an attachment to this file (Attachment E-14):

- Compiled Statistics = population statistics for all chemicals by subpopulation and age group
- Exposure by PUC = fractional dose (i.e., fraction of total dose) for each chemical by PUC and subpopulation

3. R Scripts

The following R scripts were developed and included as attachments to this file:

- Attachment E-15_SHEDS-HT Postprocessing.R = calculates (i) population statistics for the subpopulation of simulated individuals with non-zero product exposures and (ii) % contribution by PUC for each chemical
- Attachment E-16_Database_Fitting.R = fits the individual product concentration data from Holder et al. (2023) and Dewapriya et al. (2023) to a log normal distribution to obtain geometric mean and 95th percentile weight fractions; calculates a pooled geometric mean and 95th percentile for each PUC

4. References

Bennett, D.H., Furtaw Jr., E.J. 2004. Fugacity-based indoor residential pesticide fate model. Environmental Science & Technology 38, 2142-2152. https://doi.org/10.1021/es034287m

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