The High-Throughput Stochastic Human Exposure and Dose Simulation Model (SHEDS-HT)

CCTE NAMs Training Workshop

Research Triangle Park, NC

April 24 – 25, 2024

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Road Map

- PART I: SHEDS-HT Background
  - Research problem and motivation
  - SHEDS-HT Overview
  - SHEDS-HT History – how has the model been used?
- PART II: Understanding and Using the Model (R Package)
  - Understanding SHEDS-HT Terminology: Sources, Scenarios and Routes
  - Input and Output Data/Files
- PART III: Brief Demonstration/Tutorial
  - SHEDS-HT Home Directory structure and models runs, demonstration of running the CPDat V3 case study (provided with SHEDS-HT)

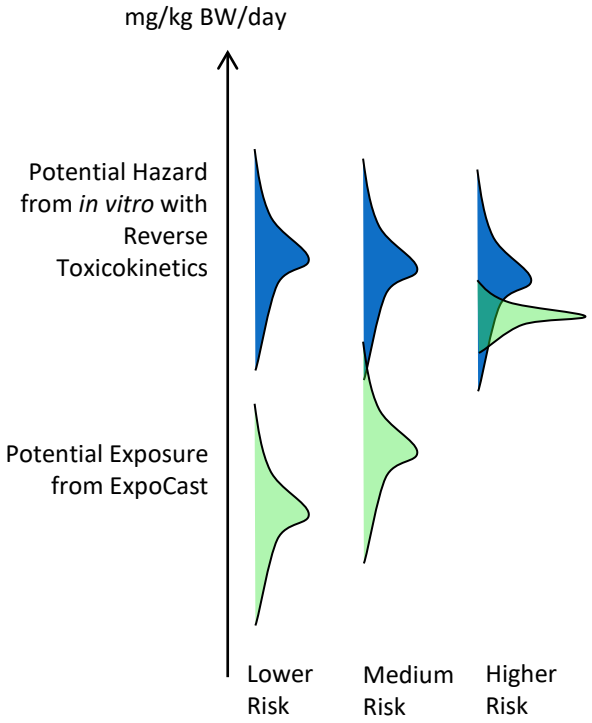
PART I: SHEDS-HT Background

Research Problem

- The timely characterization of the human and ecological risk posed by thousands of existing and emerging commercial chemicals is a critical challenge facing EPA in its mission to protect public health and the environment

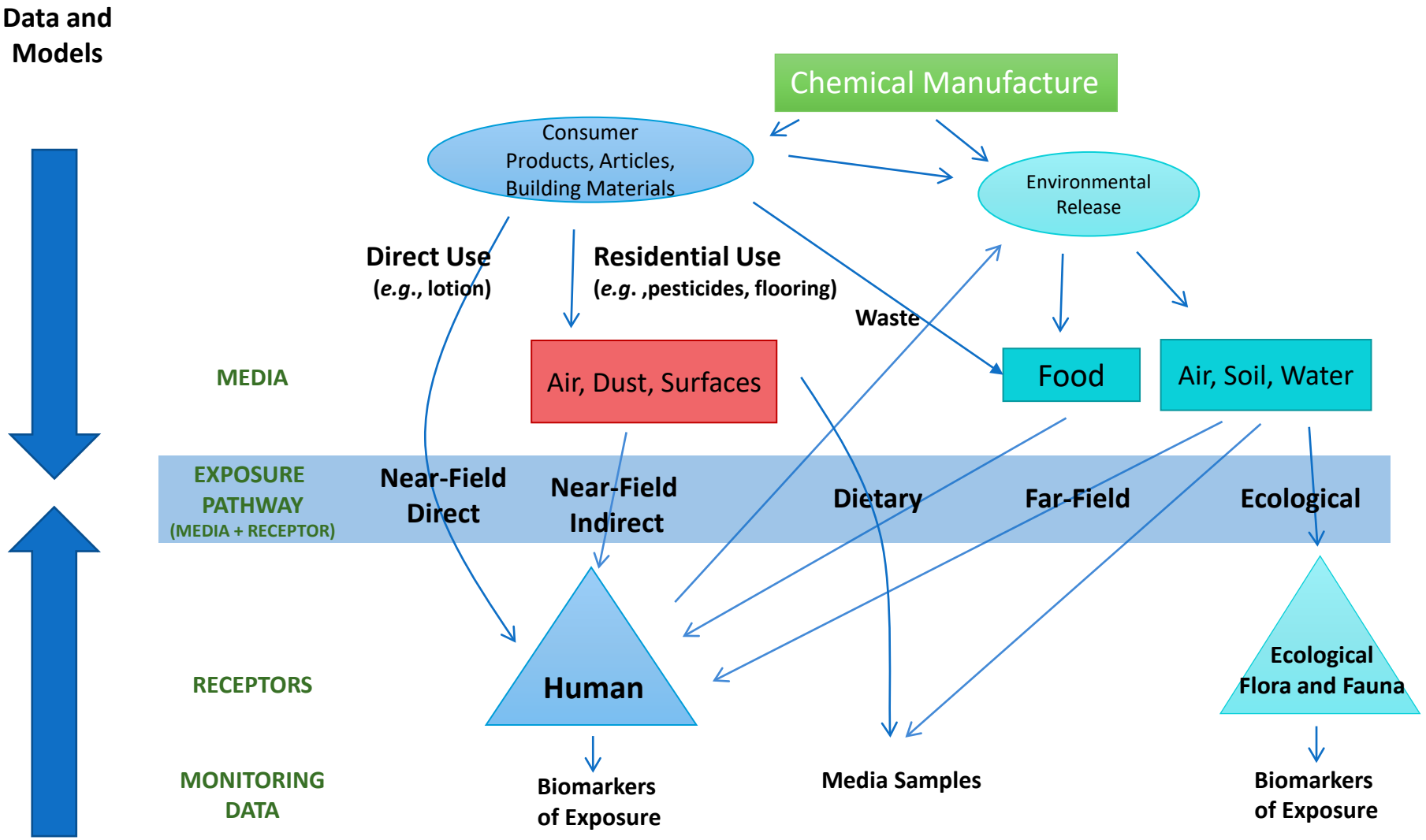
- **High throughput risk prioritization** relies on **three components** – high throughput **hazard** characterization, high throughput **exposure** forecasts, and high throughput **pharmacokinetics** (*i.e.*, dosimetry)

- While advances have been made in HT toxicity screening, evaluated exposure and dosimetry prediction methods applicable to 1000s of chemicals are needed

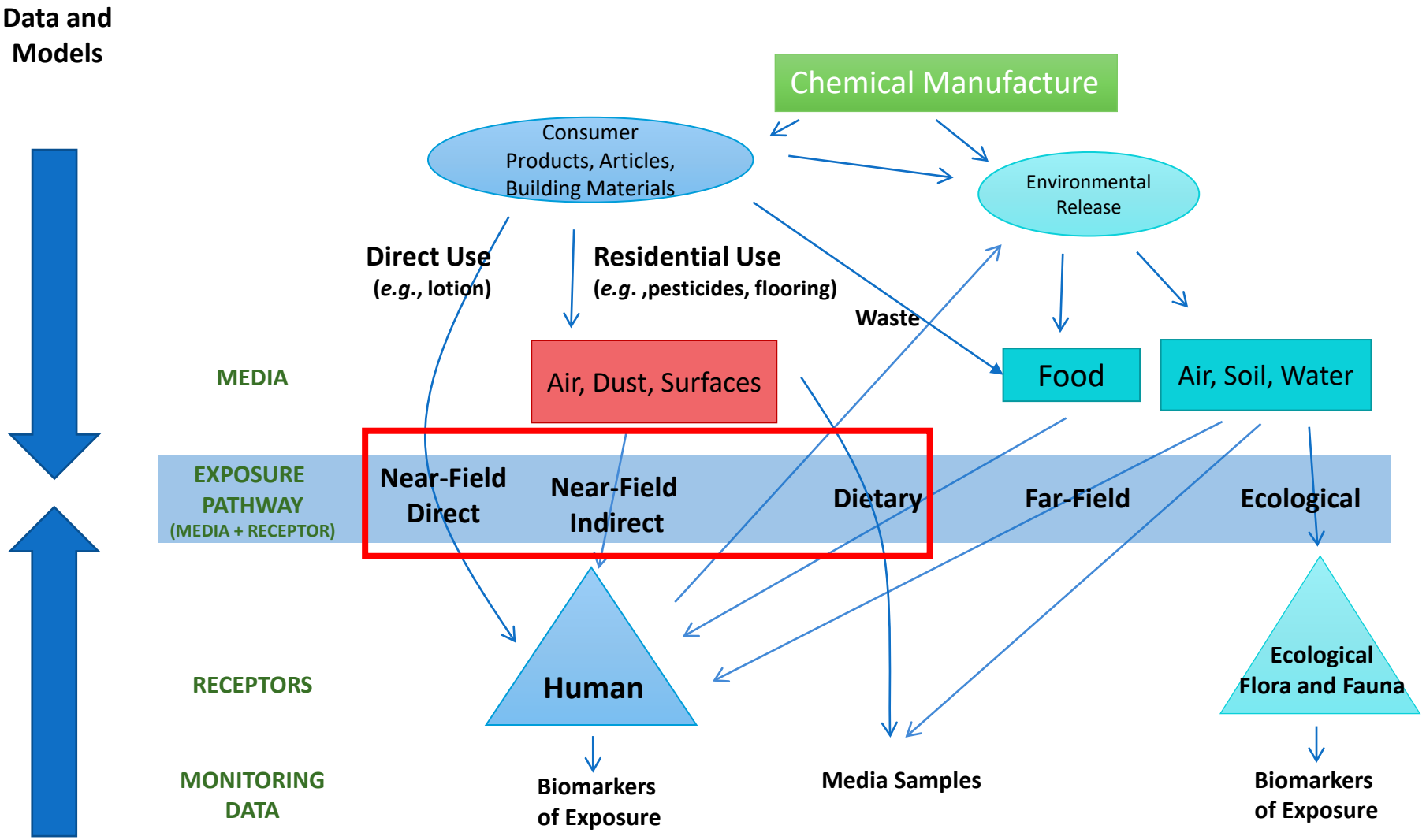


e.g. Judson *et al.,* (2011)
Chemical Research in Toxicology

Chemical Exposure Pathways



Chemical Exposure Pathways



SHEDS-HT: The Basics

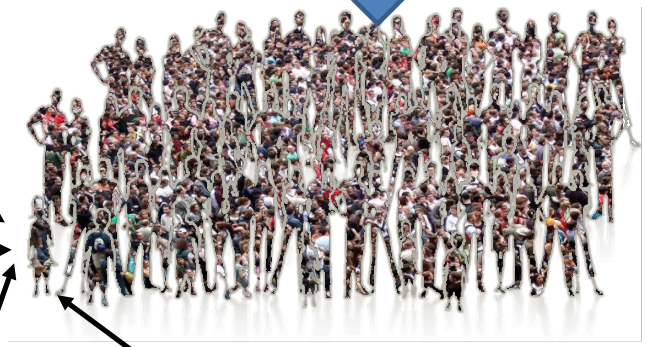
- What does the model do (in a very general sense)?
- What type of model is it?
- How has it been used in the past?
- How is the model supported, maintained, distributed, updated?

SHEDS-HT: Overview

- Stochastic Human Exposure and Dose Simulation Model (SHEDS) – High Throughput (HT)
- Produces population-level distributions of exposures to chemicals with near-field sources
- Predicts aggregate exposures to thousands of commercial chemicals in consumer products, consumer articles, and foods via inhalation, dermal, ingestion, and dietary routes in a high-throughput manner.
- General design purpose: development of HT near-field exposure predictions for use in chemical screening and prioritization

What does the model do?

Generates a simulated population and their behaviors

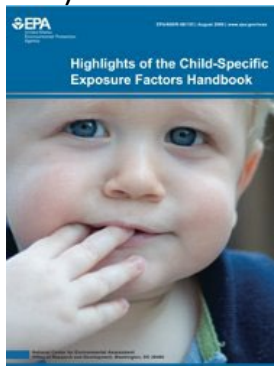


Consumer Product Use Patterns

Relevant exposure factors (e.g. weight, bathing and hand washing behaviors, hand-to mouth behaviors)

Daily-level activity diary

- Time spent in microenvironments
- Energy expenditure (ventilation)



SHEDS-HT

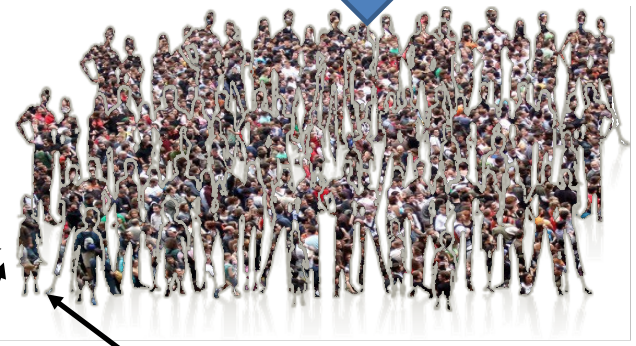
What does the model do?

Integrates chemical-specific information for sources

Chemical Residues in Foods

Chemical Ingredients and Weight Fractions

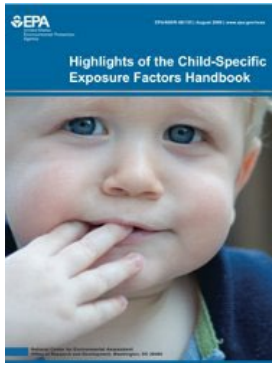
Consumer Product Use Patterns



Relevant exposure factors (e.g. weight, bathing and hand washing behaviors, hand-to mouth behaviors)

Indoor Chemical Emission from Articles

Daily-level activity diary
- Time spent in microenvironments
- Energy expenditure (ventilation)



SHEDS-HT

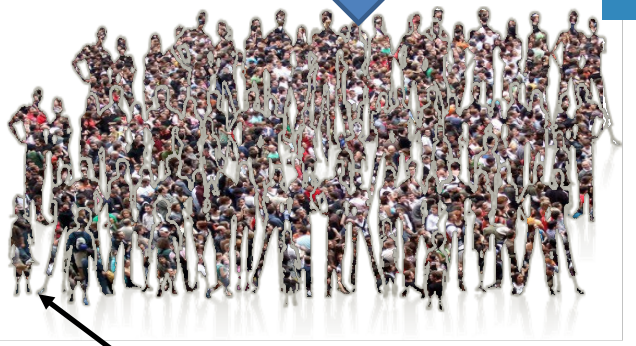
What does the model do?

Estimates resulting exposures (aggregated across sources) for individuals and population

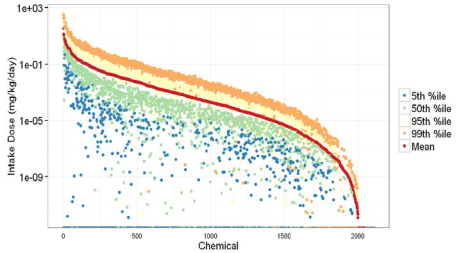
Chemical Residues in Foods

Chemical Ingredients and Weight Fractions

Consumer Product Use Patterns



Population Exposure mg/kg/day



Relevant exposure factors (e.g. weight, bathing and hand washing behaviors, hand-to mouth behaviors)

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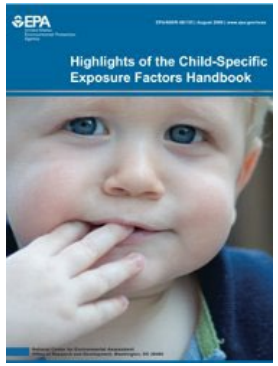
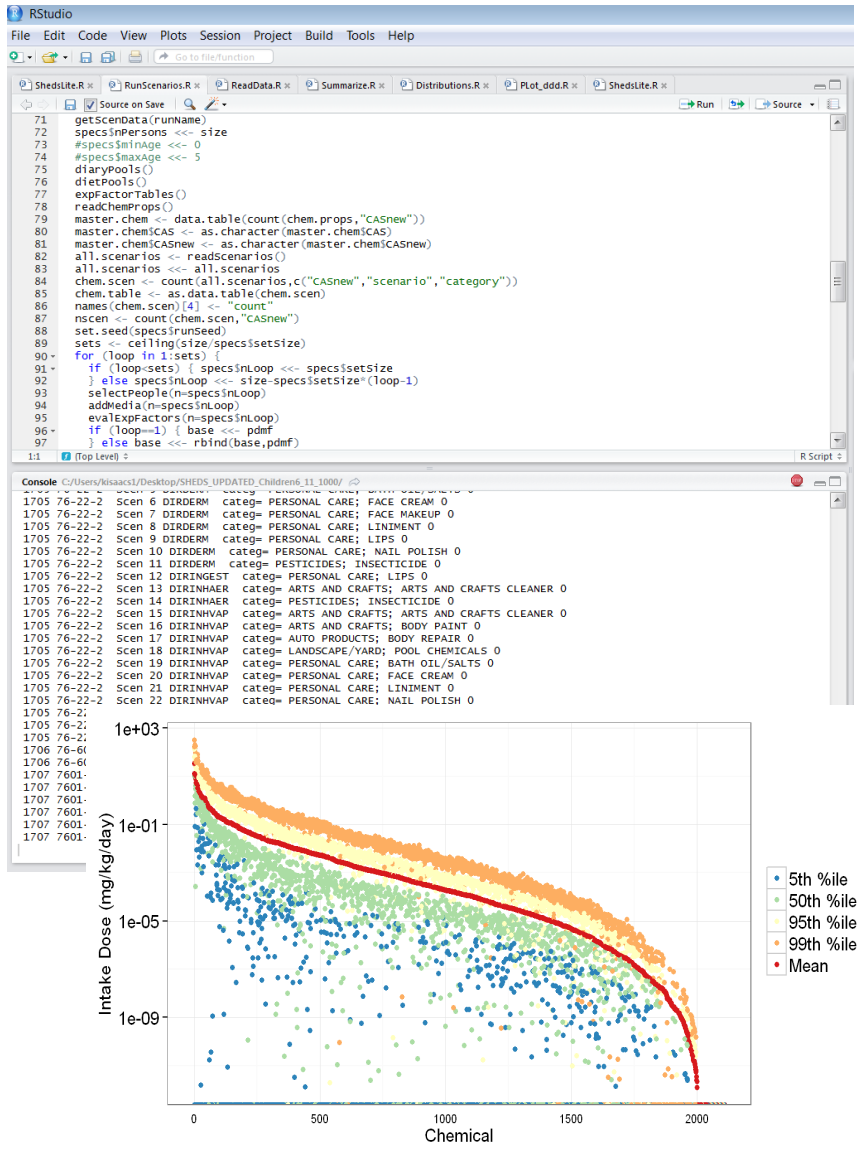


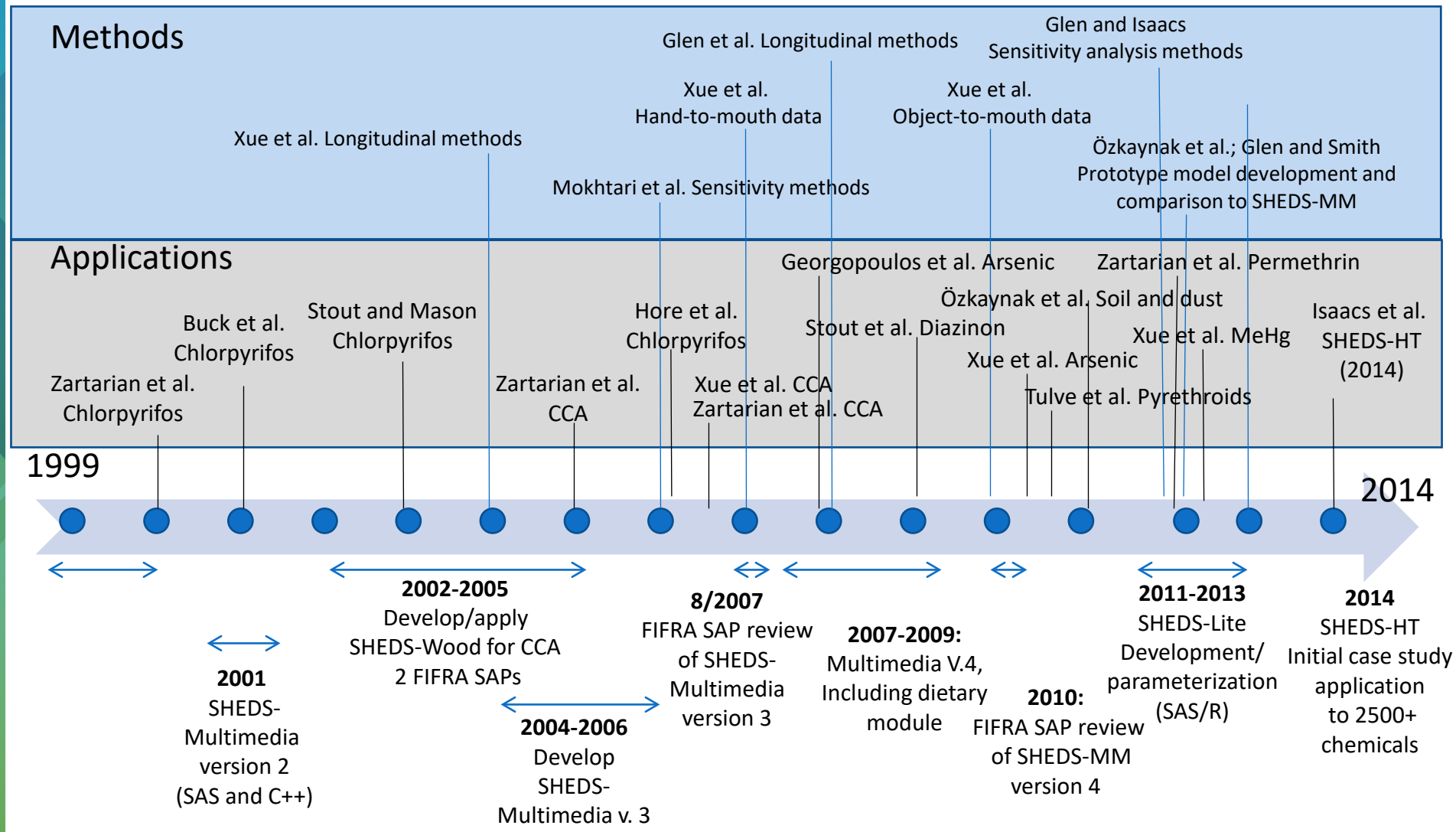
SHEDS-HT

What type of model is it?

- *High-Throughput:* Fit for specific purposes; screening and prioritization
- *Mechanistic*: Algorithms designed to reflect real physical system and its processes
- *Stochastic*: Monte-Carlo based model; takes distributions as inputs
- *Aggregate:* single chemical exposures, multi-pathway and route
- *Population-based*: simulates individuals; age-and gender differences in behaviors and data are included where possible
- *Cross-sectional*: Single day simulation predicting chemical intake doses in mg/kg/day
- Coded in the freely available R programming language
- Inputs and outputs are flexible text or CSV files



Background and History: SHEDS-Multimedia to SHEDS-HT

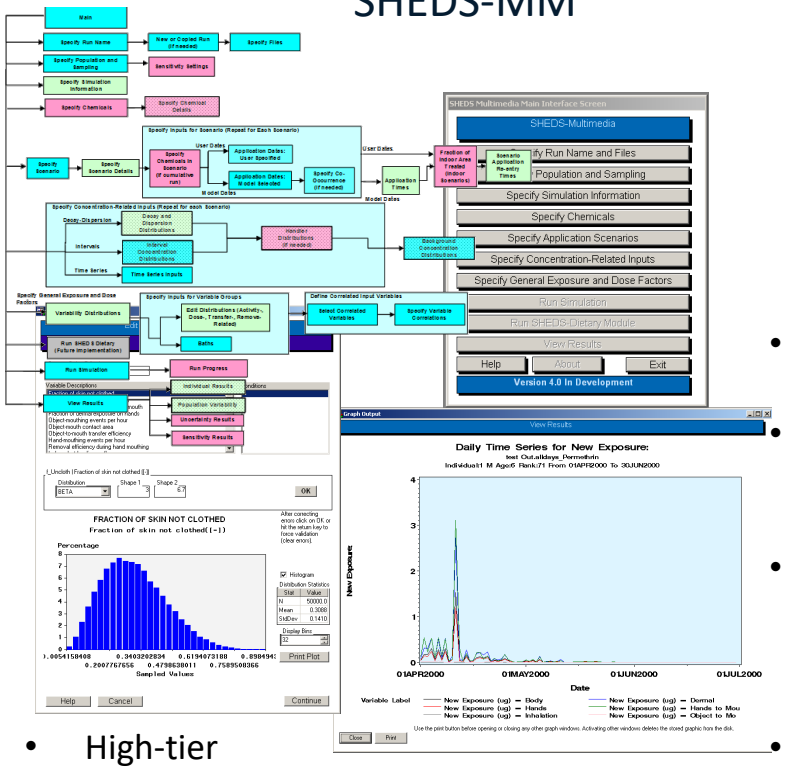


2014 - present:

SHEDS-HT applications and incorporation into EPA's ExpoCast consensus exposure predictions

SHEDS-MM to SHEDS-HT

SHEDS-MM



- High-tier
- Minute-level time resolution
- Best for single/few chemicals
- SAS-based ($$)
- Separate dietary/residential modules
- 40+ interface screens
- ~200 inputs/distributions
- Longitudinal
- Potentially long run times for large populations

- Reduced temporal resolution (daily)
- Variance decomposition based sensitivity: elimination of minor inputs
- Additional exposure scenarios (direct exposures to consumer products; emission from articles)
- Reduced version of indoor emissions fugacity module

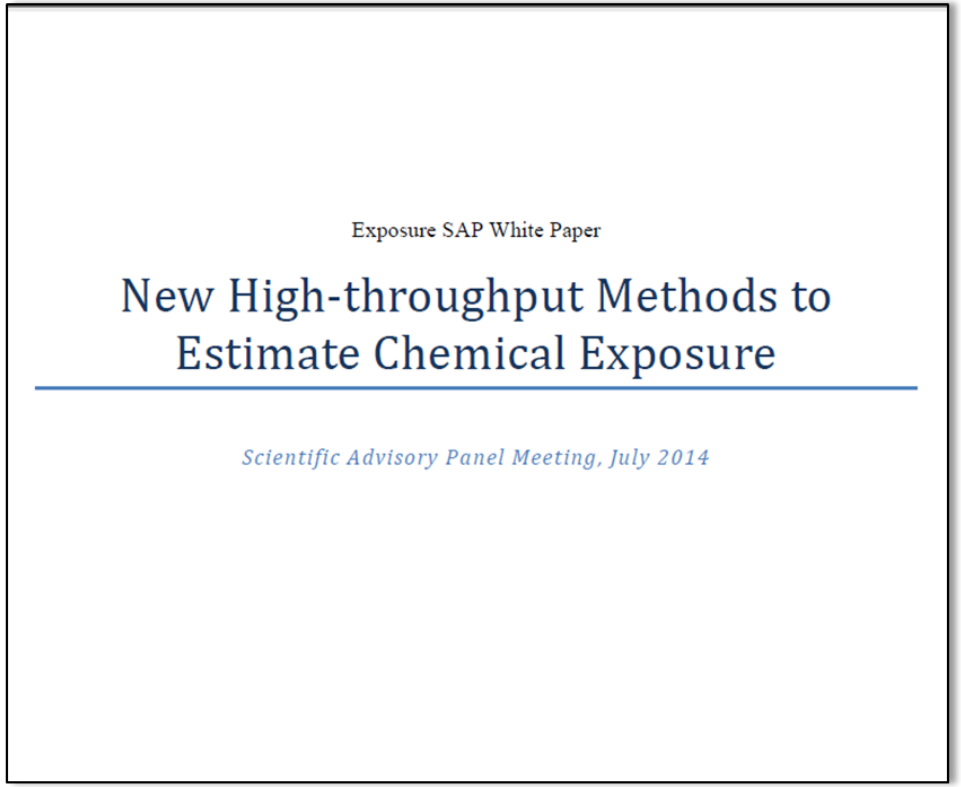
SHEDS-HT

- Low-to-mid tier
- Appropriate for 1000s of chemicals
- Retains population and life-stage information
- R-based (freely available)
- Fast execution (1000 person-days per chemical ~10 seconds)
- Combined dietary/residential: aggregate predictions
- Extendable to additional scenarios

Model Peer Review

- Model approaches favorably reviewed by July 2014 Federal Insecticide, Fungicide, Rodenticide Act (FIFRA) Scientific Advisory Panel (SAP) as part of review of Exposure Forecasting (ExpoCast) methods

- Letter peer review (2021); version of the model that responds to this peer review has been developed and is currently undergoing final QA and testing via contract
  - Estimated official release late summer 2024


Exposure SAP White Paper

New High-throughput Methods to Estimate Chemical Exposure

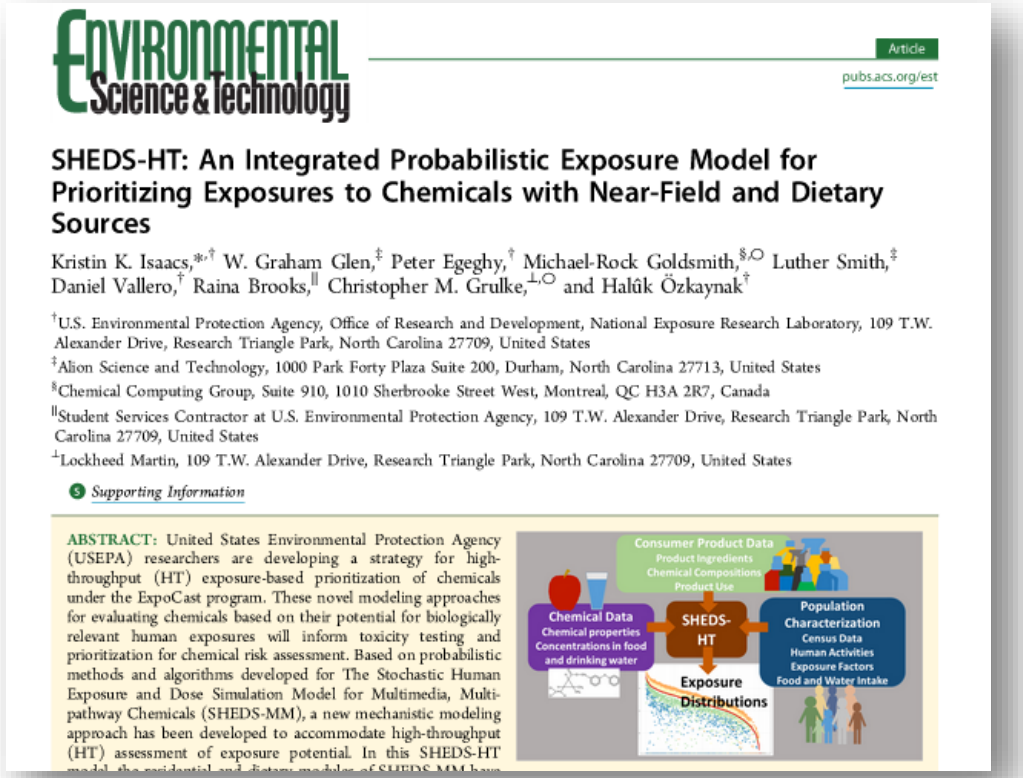
Scientific Advisory Panel Meeting, July 2014

https://federalregister.gov/a/2014-12593

Agency/Docket Numbers:
EPA-HQ-OPP-2014-0331
FRL-9910-22

How Has The Model Been Used?

- Initial SHEDS-HT publication (2014) covered general approaches and algorithms
- Included a case study to estimate population exposures for 2500 consumer product chemicals and agricultural pesticides



ENVIRONMENTAL Science & Technology

Article

pubs.acs.org/est

SHEDS-HT: An Integrated Probabilistic Exposure Model for Prioritizing Exposures to Chemicals with Near-Field and Dietary Sources

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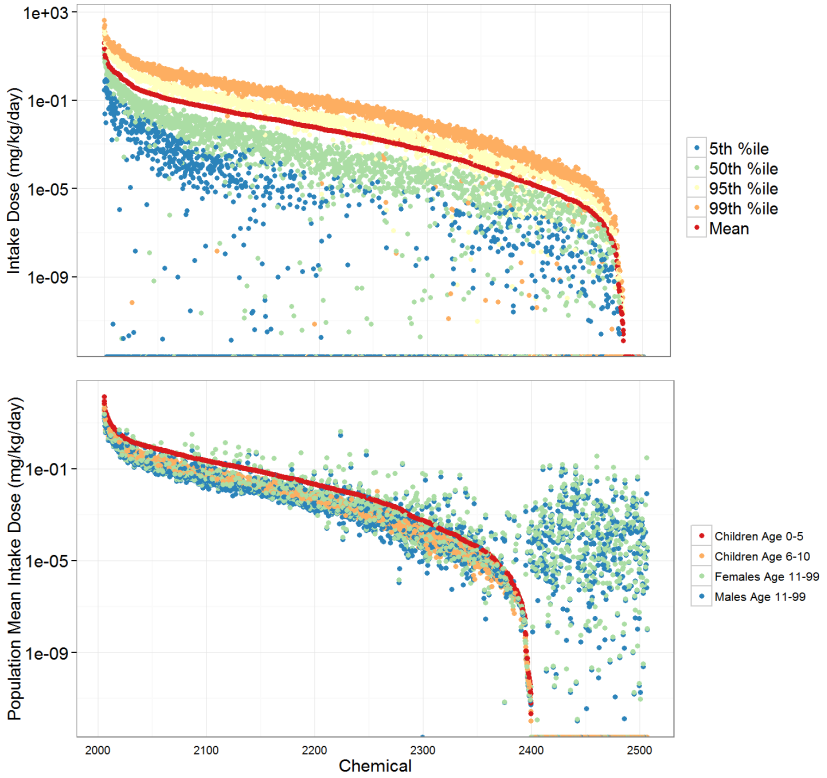
Supporting Information

ABSTRACT: United States Environmental Protection Agency (USEPA) researchers are developing a strategy for high-throughput (HT) exposure-based prioritization of chemicals under the ExpoCast program. These novel modeling approaches for evaluating chemicals based on their potential for biologically relevant human exposures will inform toxicity testing and prioritization for chemical risk assessment. Based on probabilistic methods and algorithms developed for The Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multi-pathway Chemicals (SHEDS-MM), a new mechanistic modeling approach has been developed to accommodate high-throughput (HT) assessment of exposure potential. In this SHEDS-HT



Isaacs et al., (2014)

How Has The Model Been Used?

- Development of exposure estimates for phthalates and thyroid peroxidase inhibitors (Moreau et al. 2017, Leonard et al., 2017)
- Estimation of down-the-drain chemical releases for use in ecological exposure modeling (Barber et. al, 2016)
- Exposures estimates for 10,000 product-chemical combinations to support the selection of priority products by the California Department of Toxic Substance Control (NAS, 2018)
- Incorporation of indoor VOC emissions into inventories used in air quality assessments (Qin et. al, 2020)
- Estimation of paraben exposures in personal care products and comparison to biomonitoring data (Aylward et al., 2020)
- High throughput risk and impact screening of chemicals in consumer products (Jolliet et al. 2021)

How Has The Model Been Used?

- Assessment of dietary exposures pesticides and veterinary drug residues (Luo et al., 2021, 2023)
- Assessment of dietary exposures to oxidized lipids (Maldonado-Pereira et al. 2023)
- Assessment of 1-4, dioxane exposure pathways (Dawson et al., 2022)
- **Estimation of down-the-drain releases for the Supplement to the TSCA Risk Evaluation for 1-4 Dioxane**

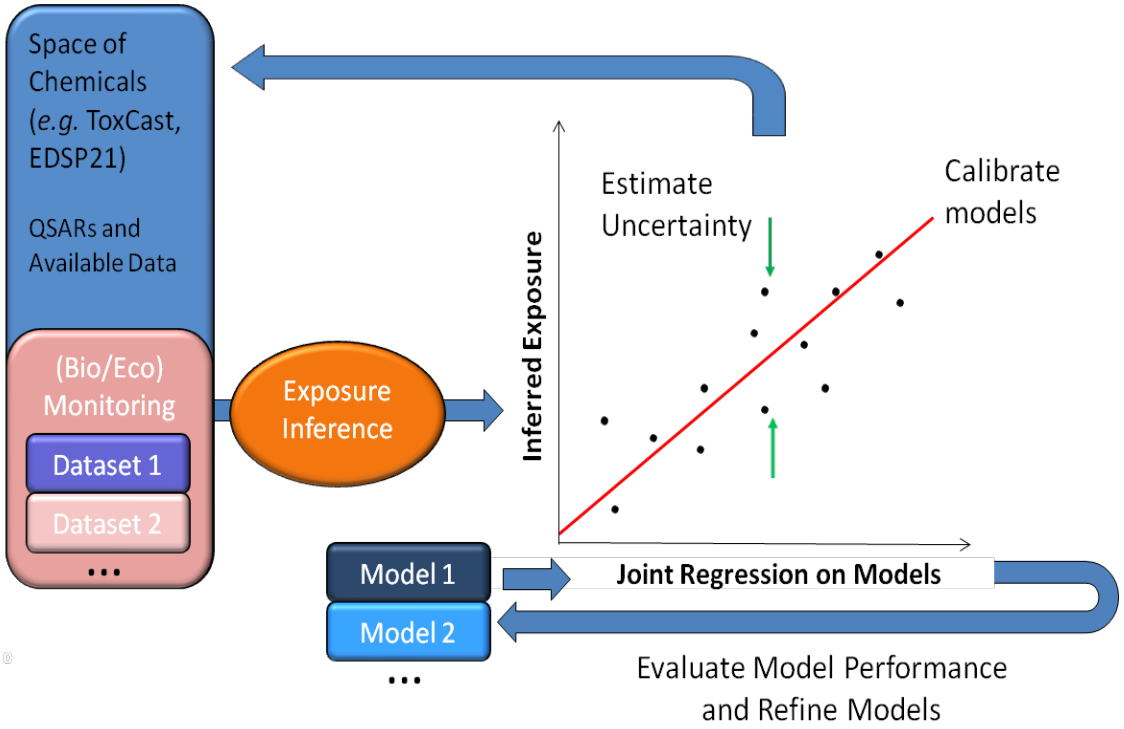
FEDERAL REGISTER
The Daily Journal of the United States Government

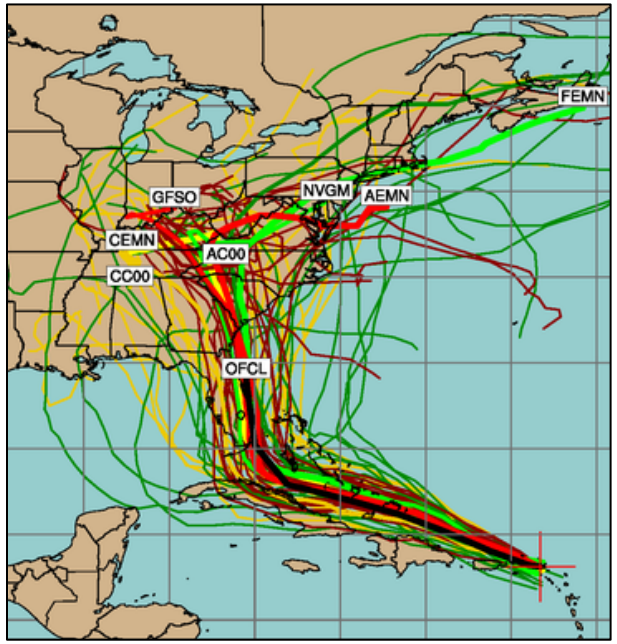
March 23, 2023

1,4-Dioxane concentrations resulting from consumer and commercial down-the-drain releases of 1,4-dioxane through publicly owned treatment works to surface water were estimated. EPA used the Stochastic Human Exposure and Dose Simulation Model (SHEDS) for high-throughput (HT) (SHEDS-HT) model (see Environ. Sci. Technol. 2014, 48, 21, 12750-12759) predictions to estimate down-the-drain disposals (Isaacs, 2014). SHEDS-HT was developed by EPA under the ExpoCast program for evaluating chemicals based on the potential for biologically relevant human exposure. This is the first TSCA risk evaluation incorporating down-the-drain estimates based on SHEDS-HT model predictions and is the first time the down-the-drain model has been used for one of the first 10 chemicals.

Consensus Exposure Predictions with the SEEM Framework

- Different exposure models incorporate **knowledge**, **assumptions**, and **data** (MacLeod et al., 2010)
- We incorporate multiple models (including SHEDS-HT) into consensus predictions for 1000s of chemicals within the **Systematic Empirical Evaluation of Models (SEEM)** (Wambaugh et al., 2013, 2014, Ring et al., 2019)
- SHEDS-HT predictions are integrated in the SEEM framework





Hurricane Path Prediction is an Example of Integrating Multiple Models

SEEM3 Collaboration

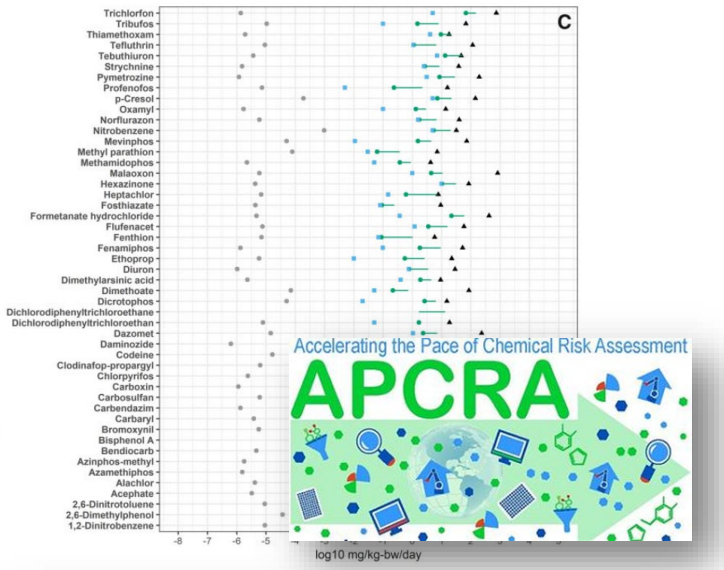
Jon Arnot, Deborah H. Bennett, Peter P. Egeghy, Peter Fantke, Lei Huang, Kristin K. Isaacs, Olivier Jolliet, Hyeong-Moo Shin, Katherine A. Phillips, Caroline Ring, R. Woodrow Setzer, John F. Wambaugh, Johnny Westgate

Predictor	Reference(s)	Chemicals Predicted	Pathways
EPA Inventory Update Reporting and Chemical Data Reporting (CDR) (2015)	US EPA (2018)	7856	All
Stockholm Convention of Banned Persistent Organic Pollutants (2017)	Lallas (2001)	248	Far-Field Industrial and Pesticide
EPA Pesticide Reregistration Eligibility Documents (REDs) Exposure Assessments (Through 2015)	Wetmore et al. (2012, 2015)	239	Far-Field Pesticide
United Nations Environment Program and Society for Environmental Toxicology and Chemistry toxicity model (USEtox) Industrial Scenario (2.0)	Rosenbaum et al. (2008)	8167	Far-Field Industrial
USEtox Pesticide Scenario (2.0)	Fantke et al. (2011, 2012, 2016)	940	Far-Field Pesticide
Risk Assessment IDentification And Ranking (RAIDAR) Far-Field (2.02)	Arnot et al. (2008)	8167	Far-Field Pesticide
EPA Stochastic Human Exposure Dose Simulator High Throughput (SHEDS-HT) Near-Field Direct (2016)	**Isaacs (2016)**	**7511**	**Far-Field Industrial and Pesticide**
SHEDS-HT Near-field Indirect (2016)	**Isaacs (2016)**	**1119**	**Residential**
SHEDS-HT Food Contact (2017)	**Biryol et al. (2017)**	**1025**	**Dietary**
Fugacity-based INdoor Exposure (FINE) (2017)	Bennett et al. (2004), Shin et al. (2012)	645	Residential
RAIDAR-ICE Near-Field (0.803)	Arnot et al., (2014), Zhang et al. (2014)	1221	Residential
USEtox Residential Scenario (2.0)	Jolliet et al. (2015), Huang et al. (2016,2017)	615	Residential
USEtox Dietary Scenario (2.0)	Jolliet et al. (2015), Huang et al. (2016), Ernstoff et al. (2017)	8167	Dietary

Ring et al., 2018

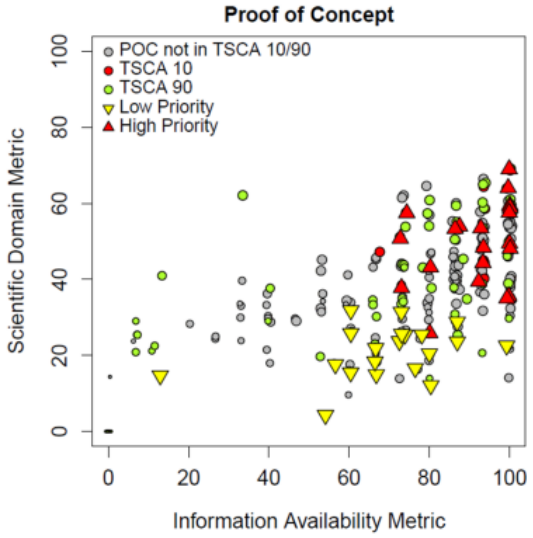
SEEM Predictions in Risk-Based Evaluation

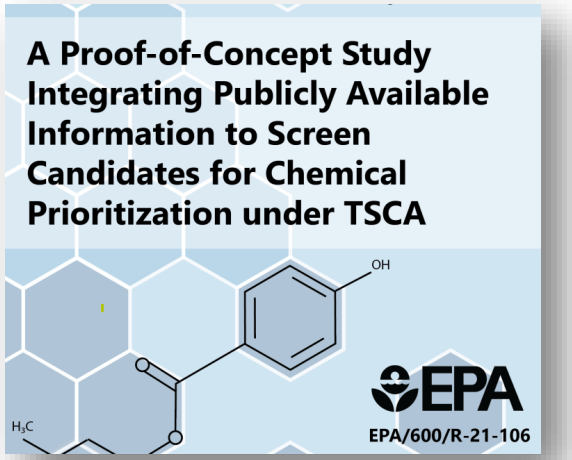
- ***Informing an international government-to-government initiative for advancing risk evaluation***



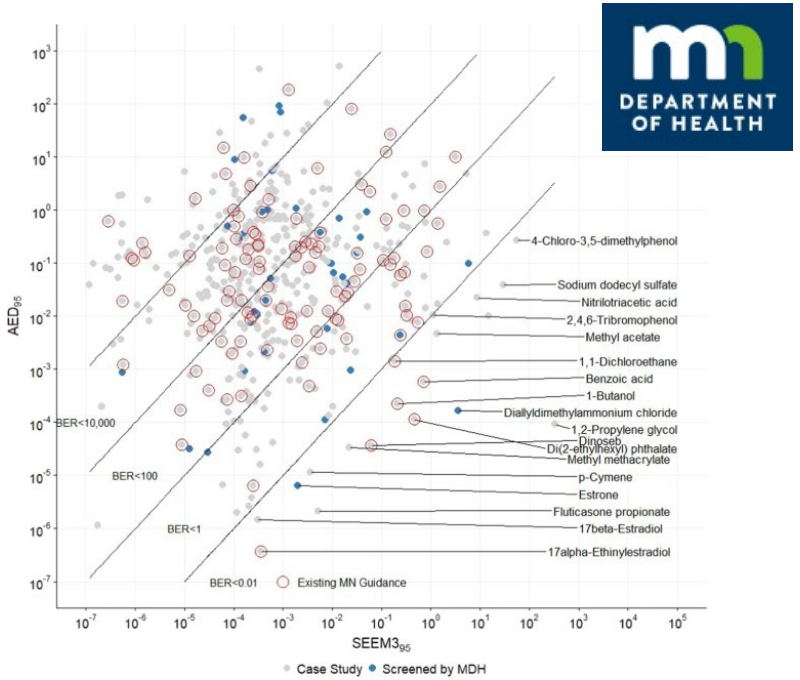
Paul-Friedman et al. (2020)

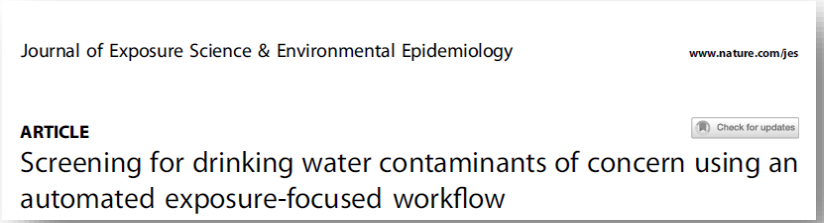
- ***Screening candidates for chemical prioritization under TSCA***





- ***Evaluating chemicals in state regulatory programs***



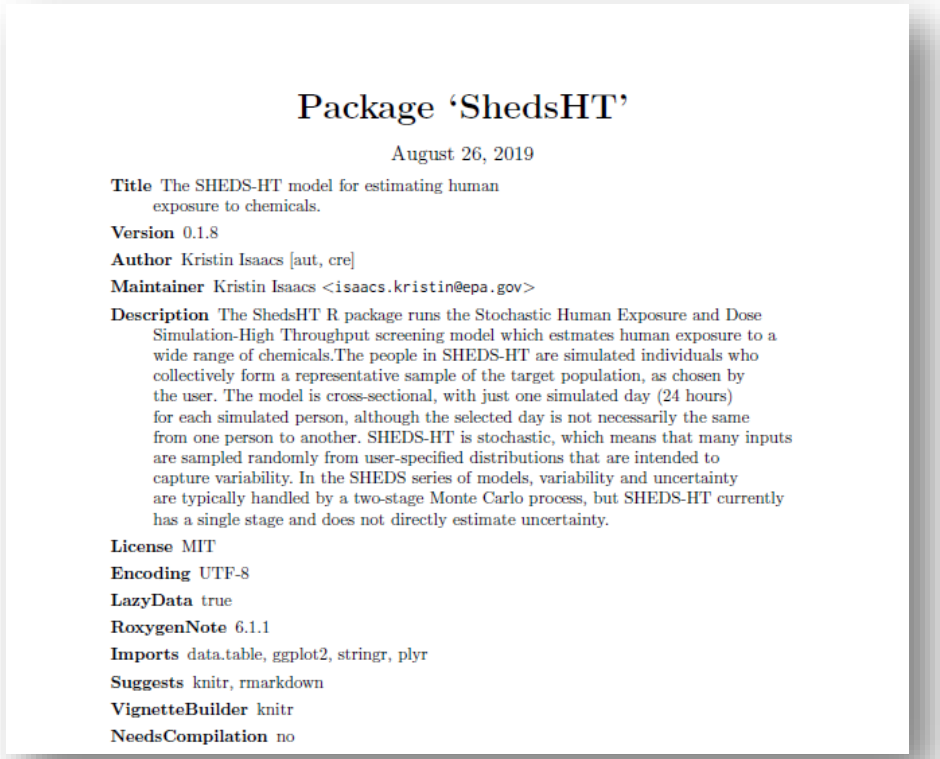


Isaacs et al., (2020)

How is the Model Supported, Maintained, Distributed, Updated?

- Development and application supported under EPA's Chemical Safety for Sustainability Program: Rapid Exposure and Dosimetry Project (ExpoCast)
- Current release is distributed as R package via EPA's GitHub site
  - https://github.com/HumanExposure/SHEDSHTRPackage

R package 'ShedsHT"



Package 'ShedsHT'

August 26, 2019

Title The SHEDS-HT model for estimating human exposure to chemicals.

Version 0.1.8

Author Kristin Isaacs [aut, cre]

Maintainer Kristin Isaacs <isaacs.kristin@epa.gov>

Description The ShedsHT R package runs the Stochastic Human Exposure and Dose Simulation-High Throughput screening model which estmates human exposure to a wide range of chemicals.The people in SHEDS-HT are simulated individuals who collectively form a representative sample of the target population, as chosen by the user. The model is cross-sectional, with just one simulated day (24 hours) for each simulated person, although the selected day is not necessarily the same from one person to another. SHEDS-HT is stochastic, which means that many inputs are sampled randomly from user-specified distributions that are intended to capture variability. In the SHEDS series of models, variability and uncertainty are typically handled by a two-stage Monte Carlo process, but SHEDS-HT currently has a single stage and does not directly estimate uncertainty.

License MIT

Encoding UTF-8

LazyData true

RoxygenNote 6.1.1

Imports data.table, ggplot2, stringr, plyr

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

- R Package with help documentation for specific functions
- Users and Technical Guide
- "Quick Start Guide"
- Default input files (e.g. population, food diaries, CPDat data in correct form)
- Example run-specific input files
- Training materials

https://github.com/HumanExposure/SHEDSHTRPackage

Recent SHEDS-HT Scientific Development

- Alignment of product categories and default consumer product input data with EPA's Chemicals and Products Database (CPDat) and Chemical Exposure Knowledgebase (ChemExpo)
- Improved handling of mass partitioning and balance across scenarios
- Better error handling and communication to user
- Improved methods for visualization of model results

PART II: Understanding SHEDS-HT Terminology (Chemicals, Sources, Scenarios, Routes, and Runs)

Chemicals

- Chemical properties need by the model can be parameterized for any compound
  - Kp: the skin permeability constant used to determine dermal absorption [cm/hr]
  - MW: molecular weight in [g/mol] of the target chemical
  - VP.Pa: vapor pressure in [Pa].
  - Log.Kow: the base ten logarithm of the octanol-water partition coefficient
  - Water.sol.mg.l: water solubility in [mg/L]
  - Half.sediment.hr: half-life in sediment [hr]; used to estimate decay of chemicals indoors (predicted by EPA's EPI-Suite Level III Fugacity model)
  - Half.air.hr: half-life in air [hr]; used to estimate decay of chemicals indoors (predicted by the EPI-Suite Level III Fugacity model)
- R package provides default values for thousands of chemicals
- EPA CompTox Dashboard provides data (including measured and modeled properties where available) for thousands of other chemicals: **https://comptox.epa.gov/dashboard**

Sources

- **A SOURCE** can be thought of as the means (or carrier) by which a chemical **enters the near-field environment**
- SHEDS-HT can handle unlimited number of sources
- SHEDS-HT allows three SOURCE types:
  - FOOD
  - PRODUCT
  - ARTICLE
- Each source in SHEDS-HT maps to one or more **SCENARIOS**

FOOD

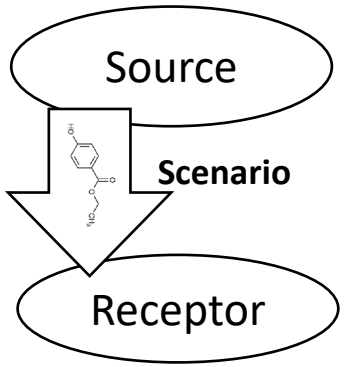
PRODUCT

(formulation)

ARTICLE

(solid)

Scenarios



- A **SCENARIO** is the mechanism by which chemical from the SOURCE comes into contact with the **receptor (usually the simulated human) resulting in exposure**
- Each **SOURCE** is mapped to one or more **SCENARIOS**
- Each **SCENARIO** has its own unique set of exposure equations
- Defines the parameters the model expects
- **SHEDS-HT** has nine unique SCENARIOS

FOOD

Food.residue: Consumption of food containing a known chemical residue

Food.migration: Consumption of food containing chemical present due to migration from packaging or other contact materials

PRODUCT

Product.direct.dermal: Direct application of chemical to skin (either purposefully or incidentally) during use of a consumer product

Product.direct.ingestion: Incidental ingestion of a consumer product during use (not including hand-to-mouth)

Product.direct.inhalationAerosol: Inhalation of aerosol during use of a consumer product

Product.direct.inhalationVapor: Inhalation of vapor during use of a consumer product

Product.Indirect: Application of consumer product to environment leading to subsequent exposures (indirect)

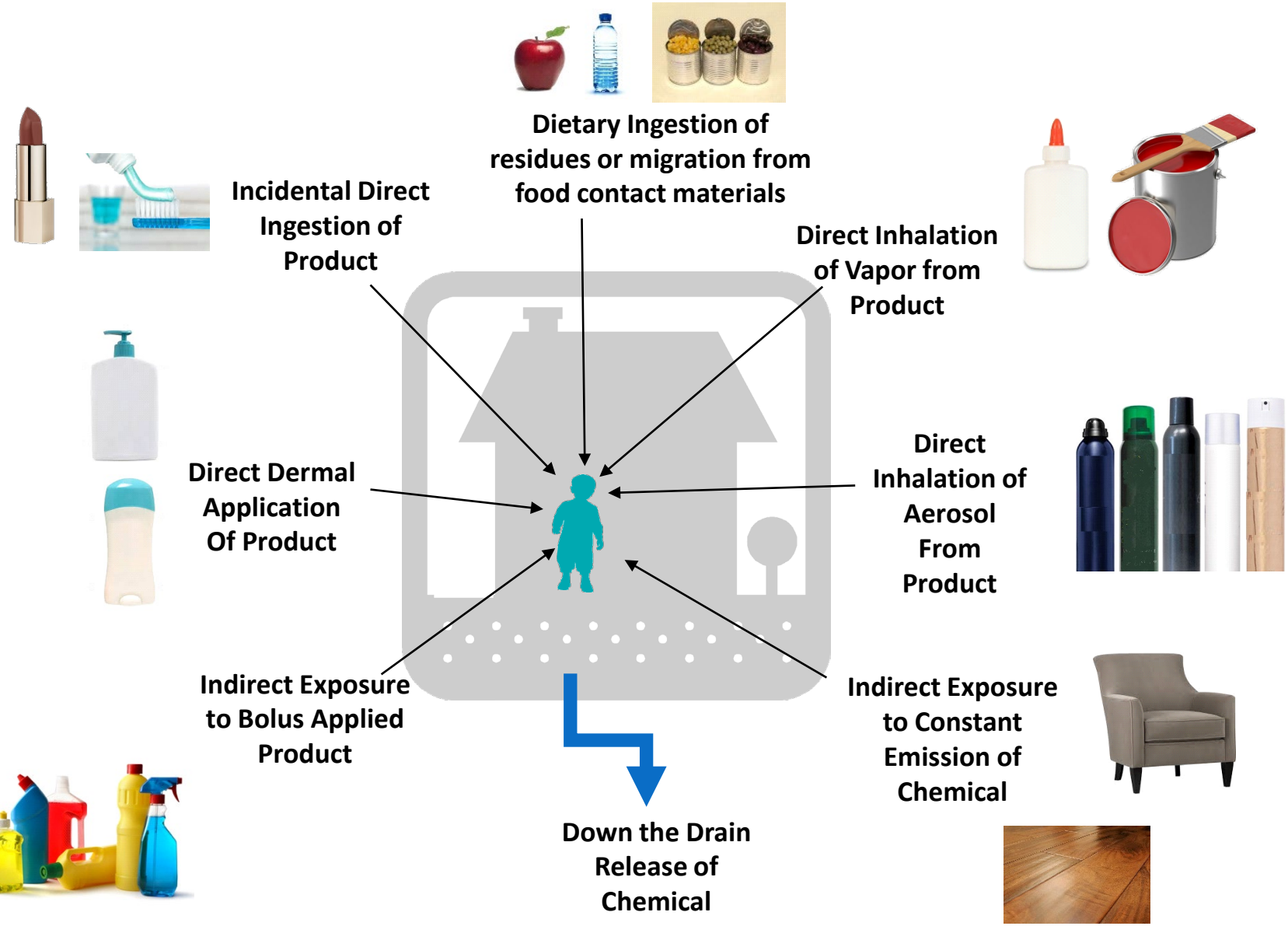
Product.downthedrain: A unique exposure scenario calculating the down the drain mass associated with use of a consumer product

ARTICLE

Article.emission: Indirect exposure due to emission of chemical from an article in the home (e.g. furnishings)

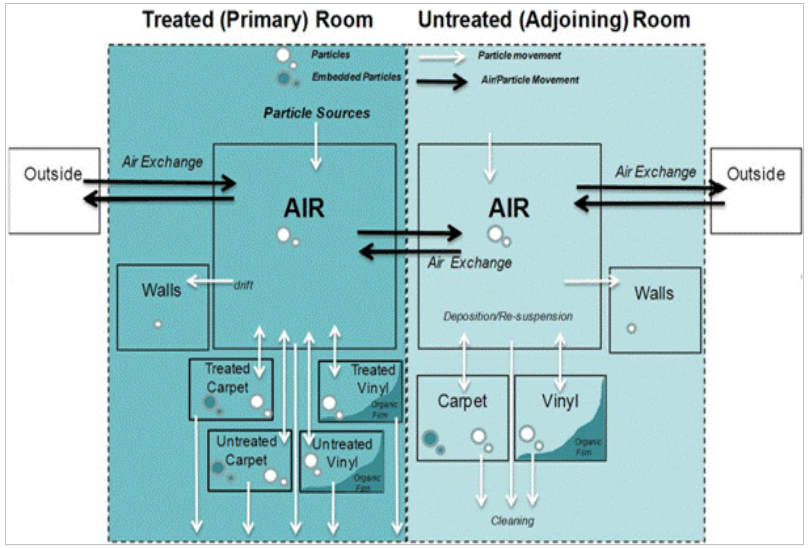
*For consumer products, both **direct** (during use) and **indirect** exposures can be modeled*

Scenarios


Dietary Ingestion of residues or migration from food contact materials
Incidental Direct Ingestion of Product
Direct Inhalation of Vapor from Product
Direct Dermal Application Of Product
Direct Inhalation of Aerosol From Product
Indirect Exposure to Bolus Applied Product
Indirect Exposure to Constant Emission of Chemical
Down the Drain Release of Chemical

Fugacity-Based Indoor Fate and Transport Model

- Indirect exposures are estimated from chemical concentrations in air and on surfaces in the home after product use
- These concentrations are estimated using a fugacity-based indoor fate and transport model
- Starting point: 10-compartment indoor fate and transport model developed for use with SHEDS-Multimedia (based on Bennett and Furtaw, ES&T, 2004)
- Reduced via variance decomposition-based sensitivity analyses (implementation of Sobol's analysis using correlations; Glen and Isaacs, *Environmental Modelling and Software*, 2012)
- Number of compartments were reduced to match SHEDS-HT (air/surfaces)
- Model is parameterized with previously developed distributions for housing characteristics and particle properties



Reduced via sensitivity analyses or use in SHEDS-HT

Critical Parameters:

Vapor Pressure

Decay Rates on Surfaces

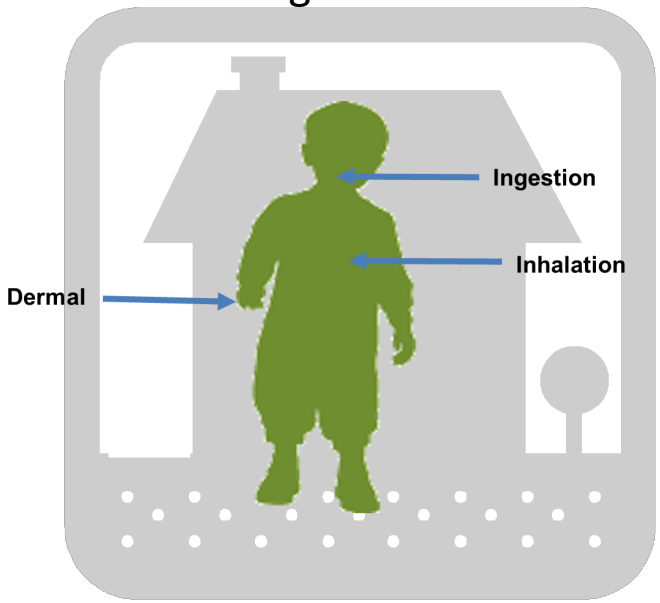
Air Exchange Rates

K_{ow}

Solubility

Route

- A **ROUTE** is the pathway by which the chemical enters the human body
  - Dermal
  - Inhalation
  - Ingestion
- Each SCENARIO results in exposure via one or more **ROUTES**
- Each ROUTE has **exposure** and **absorbed dose** values
- ROUTE exposures and doses are aggregated over SCENARIOS for each SOURCE and over each SOURCE
- ROUTES each have an absorption fraction, all combine to get absorbed dose



Route

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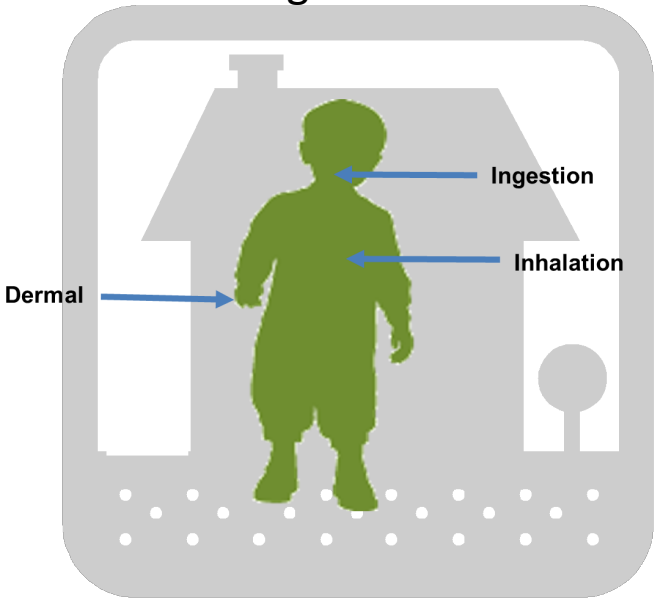
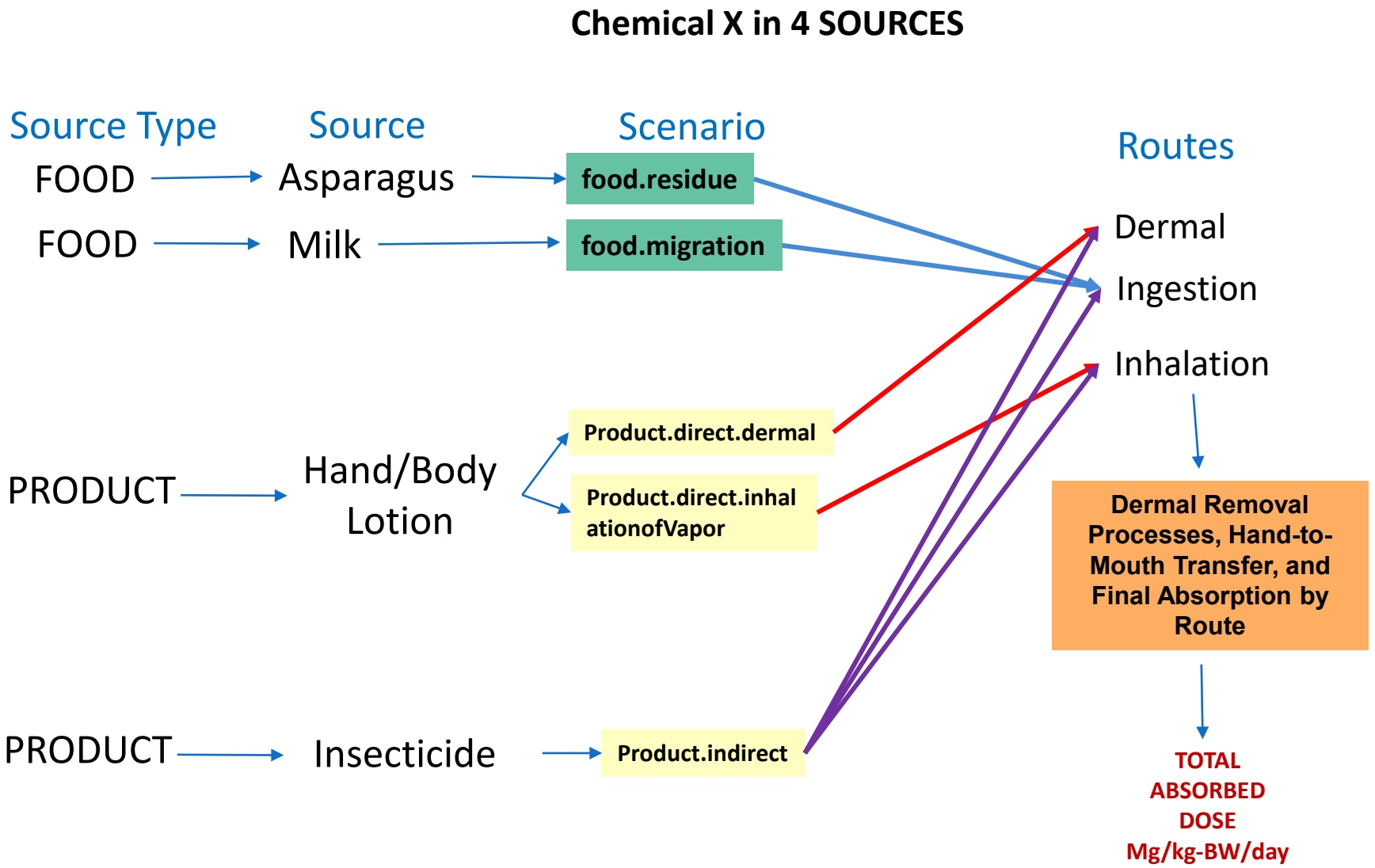
- ROUTE exposures and doses are aggregated over SCENARIOS for each SOURCE and over each SOURCE
- ROUTES each have an absorption fraction, all combine to get absorbed dose

Food.migration	Ingestion
Product.direct.dermal	Dermal, Ingestion
Product.Indirect	Dermal, Ingestion, Inhalation
Product.direct.inhalationVapor	Inhalation



Example of Linkage Chemicals, Sources, Scenarios, and Routes in a SHEDS-HT Run

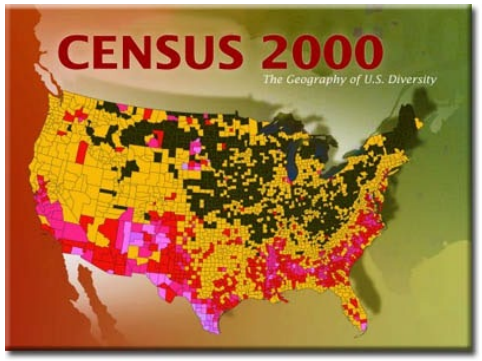


SHEDS-HT General Input Files (Not Source-Specific)

- **Default data provided**

File	Description	Source for Default Information
Activity Diary File	Daily location (time spent in microenvironments) and activity (physical activity index PAI, a time-averaged metabolic equivalent) information for each age- and gender-specific CHAD diary	Calculated from USEPA's CHAD
Chemical Property File	Chemical-specific property information by CAS number	Derived from EPA's OPERA QSARs and Epi-SUITE application
Dietary Diary File	Daily mass of food group (by default crop group) consumed by individuals	Calculated from NHANES-WWEIA food diaries
Exposure Factor File	Distributions for various human exposure factors	From Exposure Factors Handbook and analysis of other models
Fugacity File	Distributions for house variables needed for fugacity modeling	Mainly developed from Bennett and Furtaw (original indoor fate and transport model)
Media File	List of media in each micro that may contain chemicals	N/A
Physiology File	Body mass, height, and basal metabolic rate distributions or regressions by age/gender cohort	Developed from CDC's NHANES
Population File	Number of individuals in US in each age age/gender cohort	2000 US Census

Population Generation



Male, age 4

Match age and gender

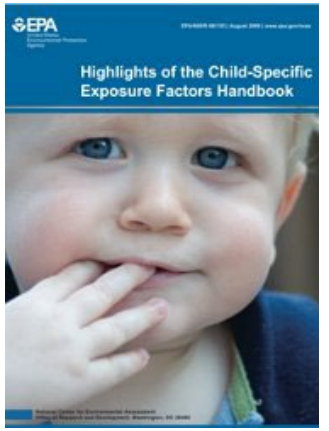
Relevant exposure factors (e.g. weight, bathing and hand washing behaviors, hand-to-mouth behaviors)

Daily-level activity diary

- Time spent in microenvironments
- Energy expenditure (ventilation)

Daily-level food diary (grams consumed per food group)

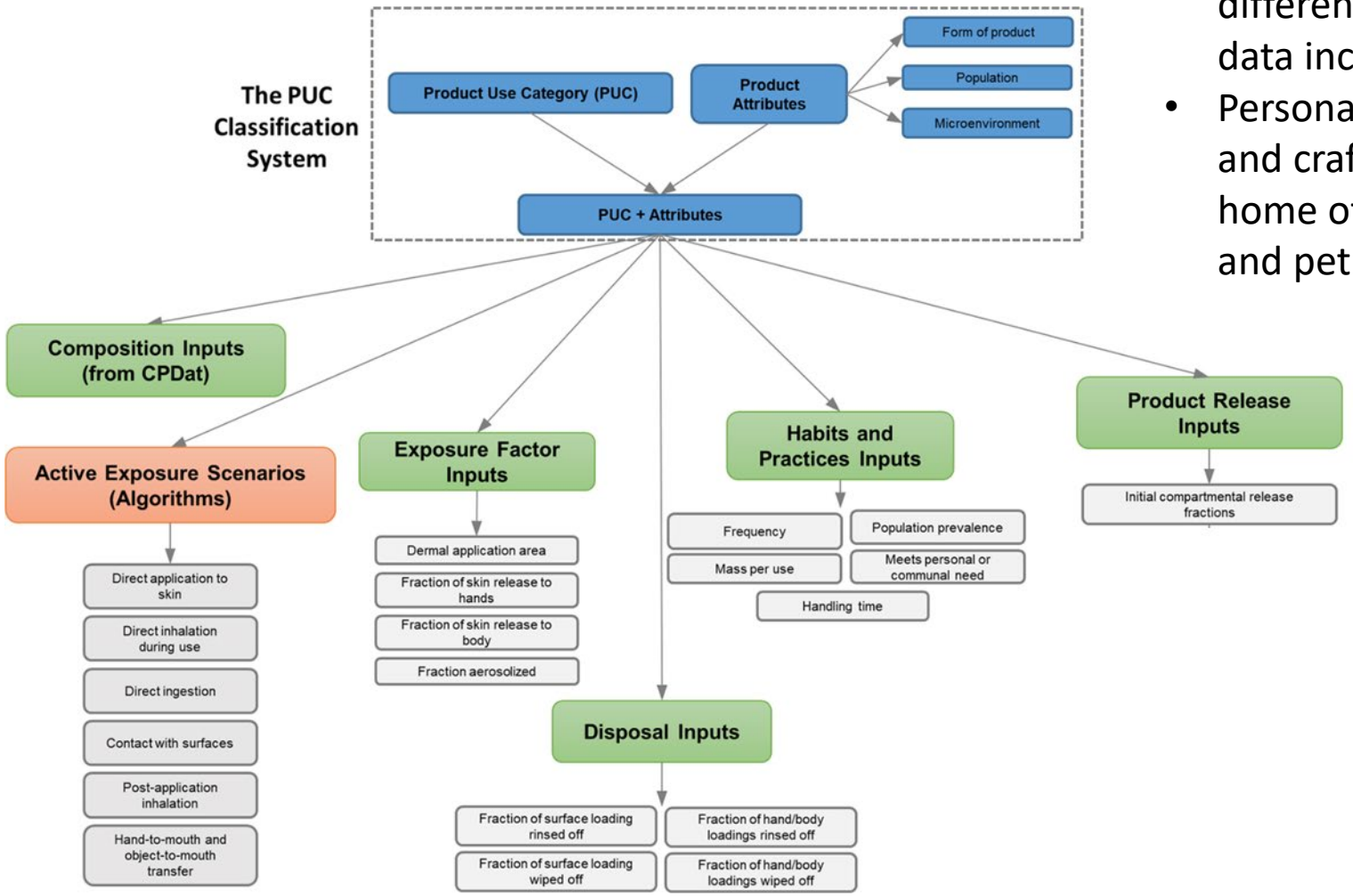
nhanes



SHEDS-HT Source-Specific Input Files

- **Source-Scenario file**
  - Which exposure scenarios are active for each source?
- **Source-Variables file**
  - Required parameter (variable) values associated with each source
  - For consumer product sources, these are consumer use patterns
    - **Default data provided**
- **Source-Chemicals file**
  - Specific chemicals associated with each source and their required parameters
  - For consumer product sources, these are consumer product chemical prevalences and weight fractions
    - **Default data provided (CPDat V1 and V3)**

Product Sources in SHEDS-HT



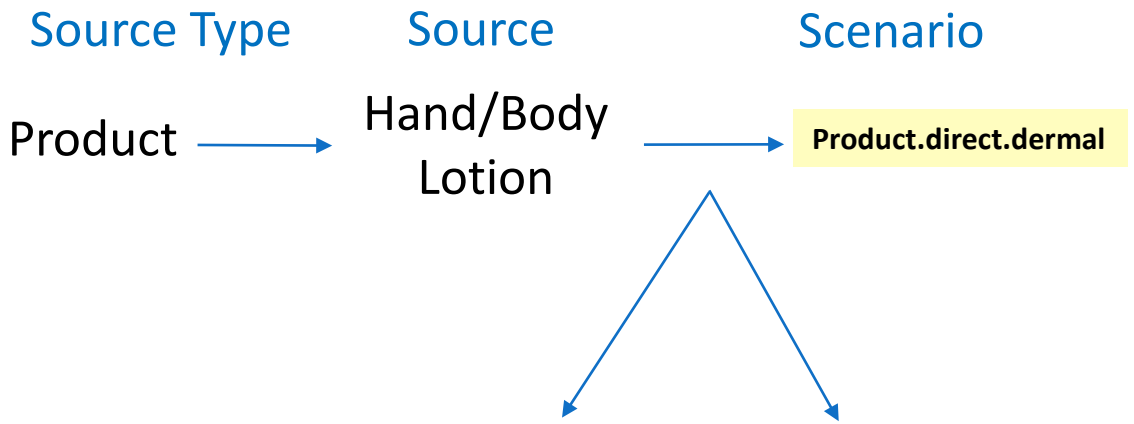
- Product categories provide linkages to critical input parameters
- SHEDS-HT can handle > 300 different product categories (default data included)
- Personal and household care, arts and crafts, home maintenance, home office, landscape and yard, and pet products included

Isaacs et al., 2020

Source-Variable Data for SHEDS-HT Default Product Categories

- Frequency of use (per year)
- Population prevalence (% households using product)
- Mass per use (g)
- Developed from available data where available
  - EPA Exposure Factors Handbook (multiple studies)
  - Other published studies (e.g. Study of Use of Products and Exposure Related Behavior, UC Davis)
  - Defaults from other screening level models (EFAST Consumer Module; ConsExpo)
- Best guess assumptions made when no data available using expert judgement

Parameterization of Consumer Product Sources



Set on Source-Scenario file

Source-Variable File Parameters

use.prev	Fraction of population using the source
use.freq	Number of times per year the source is used
mass	Mass in grams of product per use
f.contact	Fraction of product mass contacting skin
f.residual	Fraction of contacting mass remaining on skin after product use

- ***Used for all chemicals in source***
- ***Used by one or more scenarios***
- ***If missing, SHEDS writes error informing of missing info***

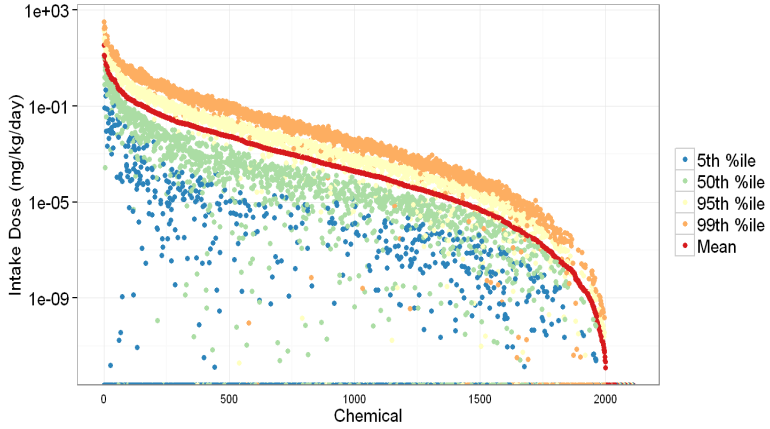
Source-Chemical File Parameters

chem.prev	Likelihood (probability between 0-1) this source type contains the chemical of interest
f.chemical	Fraction of product weight that is this chemical (if not zero)

- ***Indexed by CASRN or other ID***
- ***If missing, chemical(s) not run***
- ***If present, chemicals are run***

SHEDS-HT Outputs

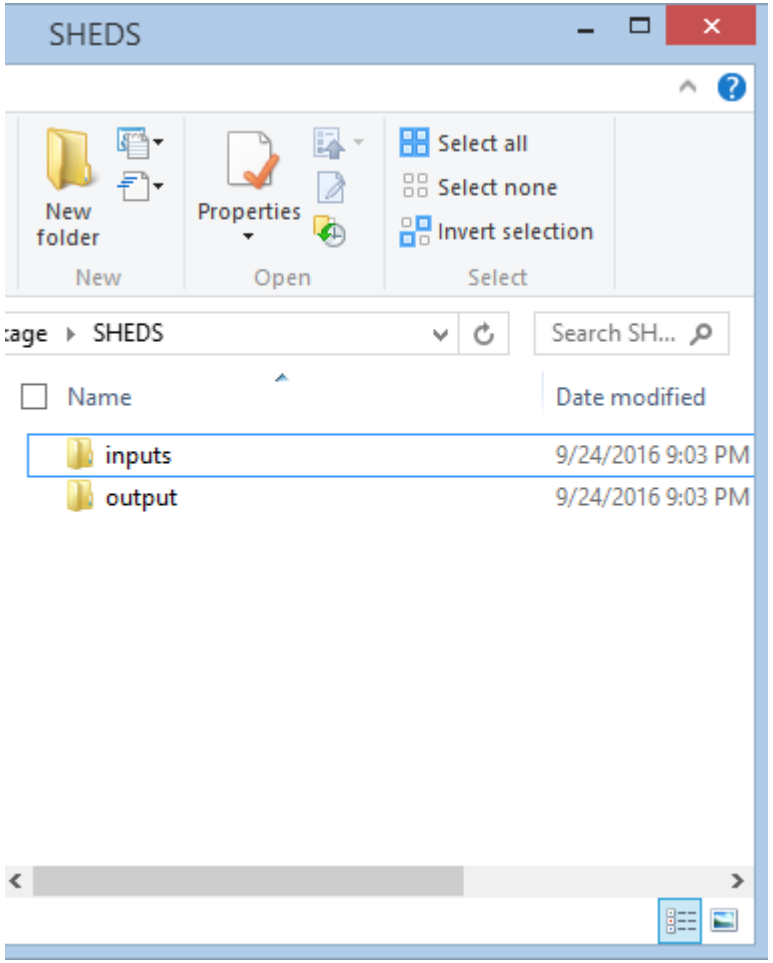
- **Individual Results**
  - Individual exposures by route
- **Source Results**
  - Mean contribution of different products and scenarios
- **Population Results**
  - Population statistics by cohort (Total, M>F, age groups, women of childbearing age) for select exposure/dose metrics



		exp.dermal	exp.ingest	exp.inhal	dose.inhal	dose.intake	abs.dermal.ug	abs.ingest.ug	abs.inhal.ug	abs.tot.ug	abs.tot.mgkg	ddd.mass
Statistic	Cohort	ug/day	ug/day	ug/m3	ug/day	mg/kg/day	ug/day	ug/day	ug/day	ug/day	mg/kg/day	g/day
0.50%	Total	0	0.45274	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0
1%	Total	0	0.45274	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0
2.50%	Total	0	0.518785	0	0	1.53E-05	0	0.353257	0	0.355344	7.44E-06	0
5%	Total	0	0.71579	0	0	1.96E-05	0	0.439642	0	0.443794	1.14E-05	0
10%	Total	0	0.951564	2.00E-06	1.00E-05	2.41E-05	0	0.726728	2.00E-06	0.76502	1.32E-05	0
15%	Total	2.097236	1.225137	1.00E-05	7.00E-05	2.62E-05	0.000189	0.870716	1.10E-05	0.894217	1.47E-05	0
20%	Total	3.605379	1.626264	1.90E-05	0.000129	2.97E-05	0.000556	1.093802	2.10E-05	1.144045	1.69E-05	0
25%	Total	6.147302	1.735642	2.70E-05	0.000175	3.30E-05	0.000744	1.325966	2.80E-05	1.384025	2.16E-05	0
30%	Total	9.721634	1.925034	2.90E-05	0.000218	3.88E-05	0.001228	1.464601	3.50E-05	1.47233	2.58E-05	0
40%	Total	15.224515	2.209967	5.50E-05	0.000358	5.49E-05	0.002051	1.670117	5.70E-05	1.710725	3.15E-05	0
50%	Total	25.134264	2.650664	9.40E-05	0.000716	6.96E-05	0.002787	2.047625	0.000115	2.116674	3.77E-05	0
60%	Total	36.382989	3.221718	0.000119	0.000912	9.38E-05	0.004416	2.284749	0.000146	2.39075	4.84E-05	0
70%	Total	64.143953	3.892597	0.000191	0.001507	0.000117291	0.00838	2.795248	0.000241	2.993058	6.68E-05	0
75%	Total	84.744533	4.169869	0.000317	0.002052	0.000126251	0.010753	3.019018	0.000328	3.239403	7.25E-05	0
80%	Total	134.414926	4.60987	0.000377	0.002674	0.000148092	0.021987	3.237884	0.000428	3.729817	8.84E-05	0

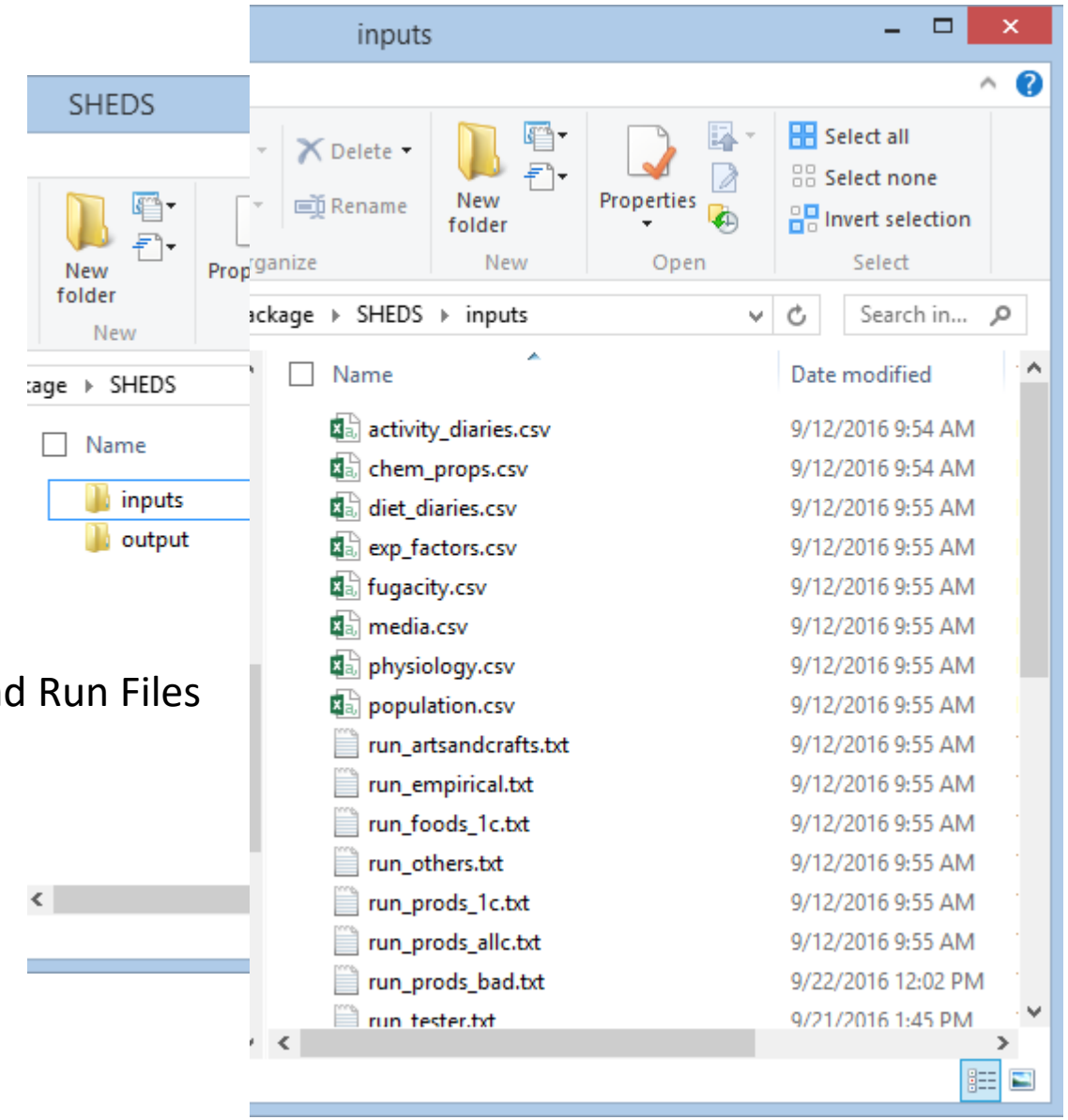
PART III: SHEDS-HT Home Directory Structure, Setting Up SHEDS, and Running the Model

SHEDS Home Directory Structure



- We will cover set-up from R package in Demo

SHEDS Home Directory Structure

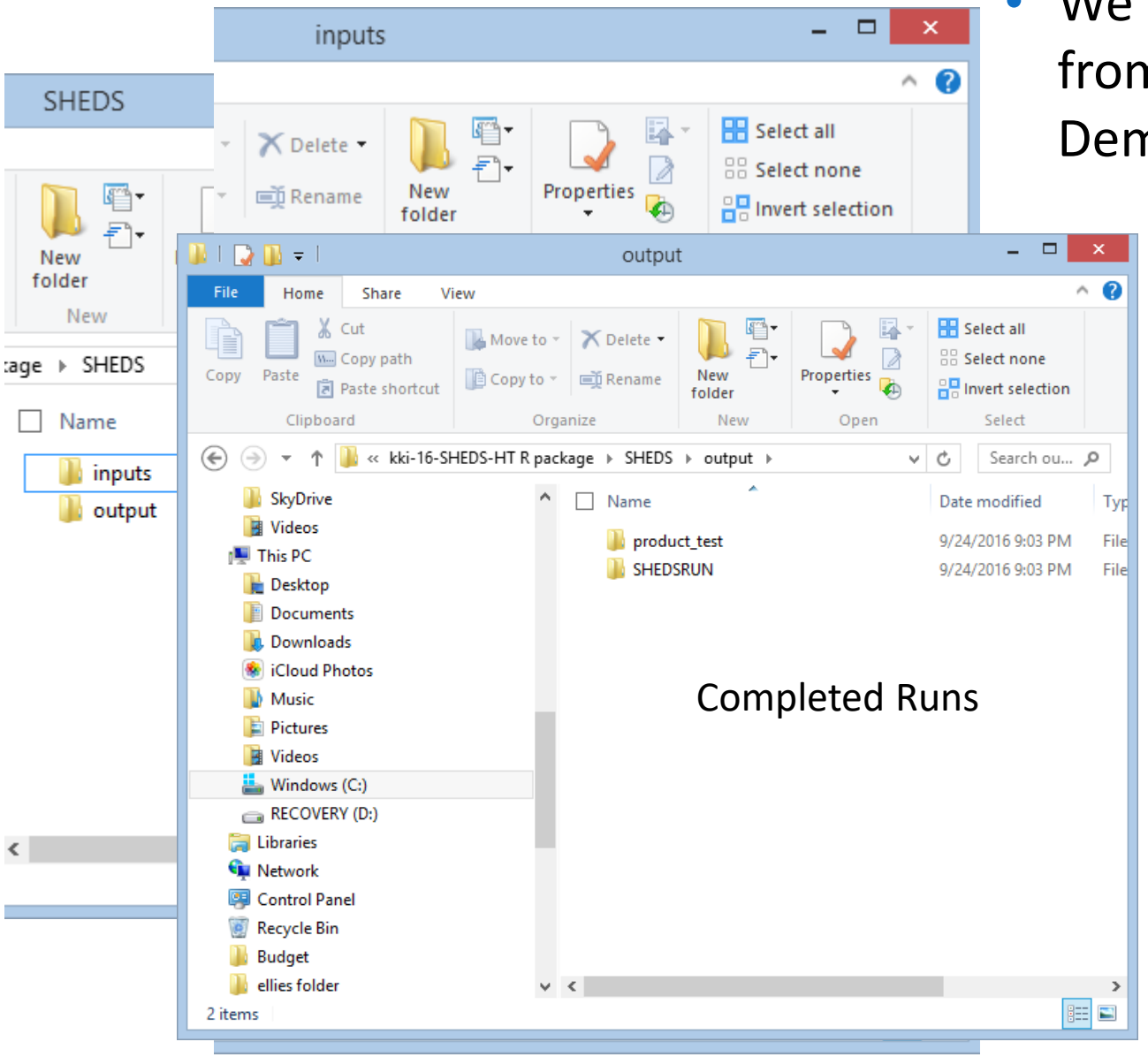


Input and Run Files

- We will cover set-up from R package in Demo

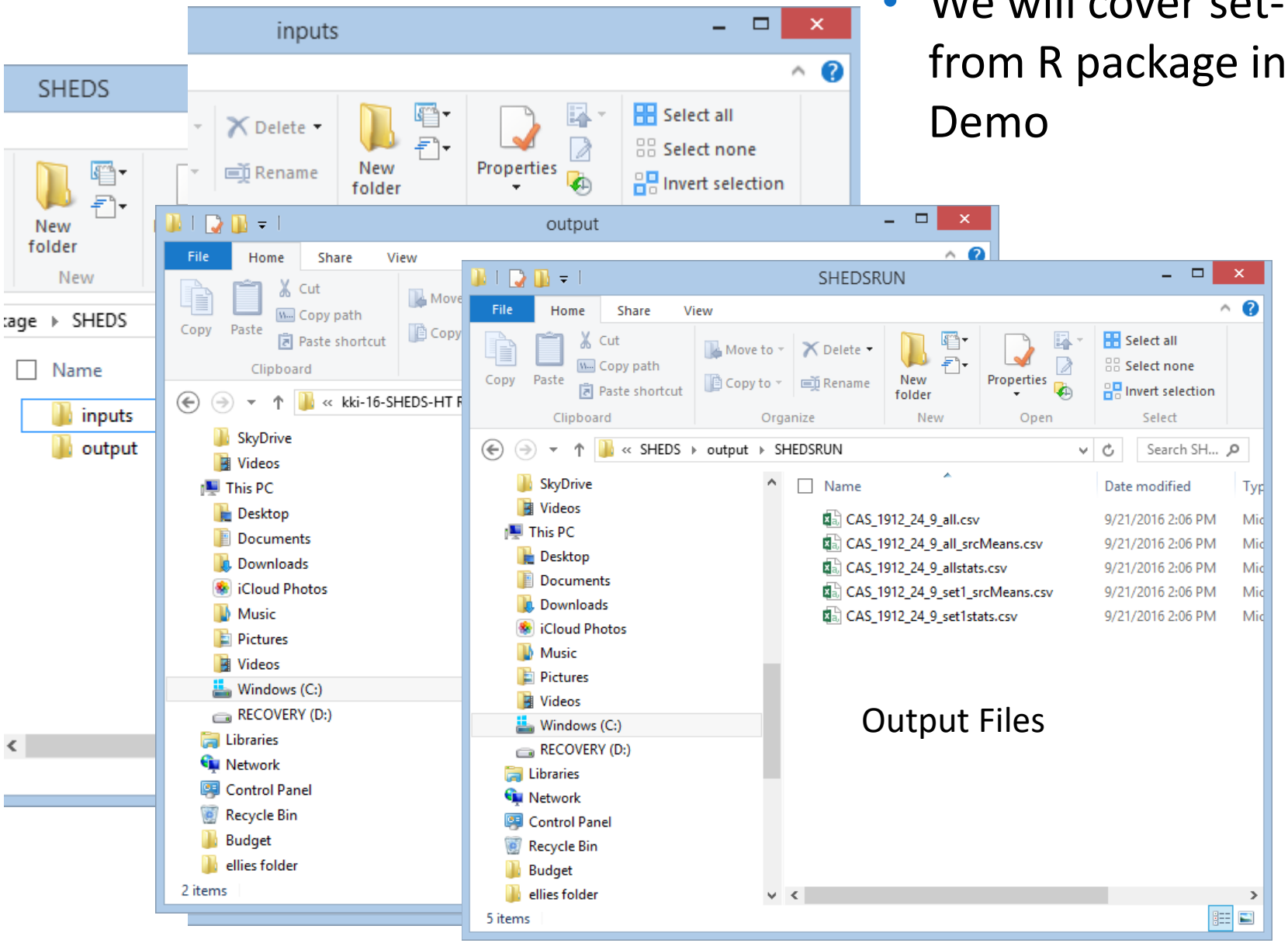
SHEDS Home Directory Structure

- We will cover set-up from R package in Demo



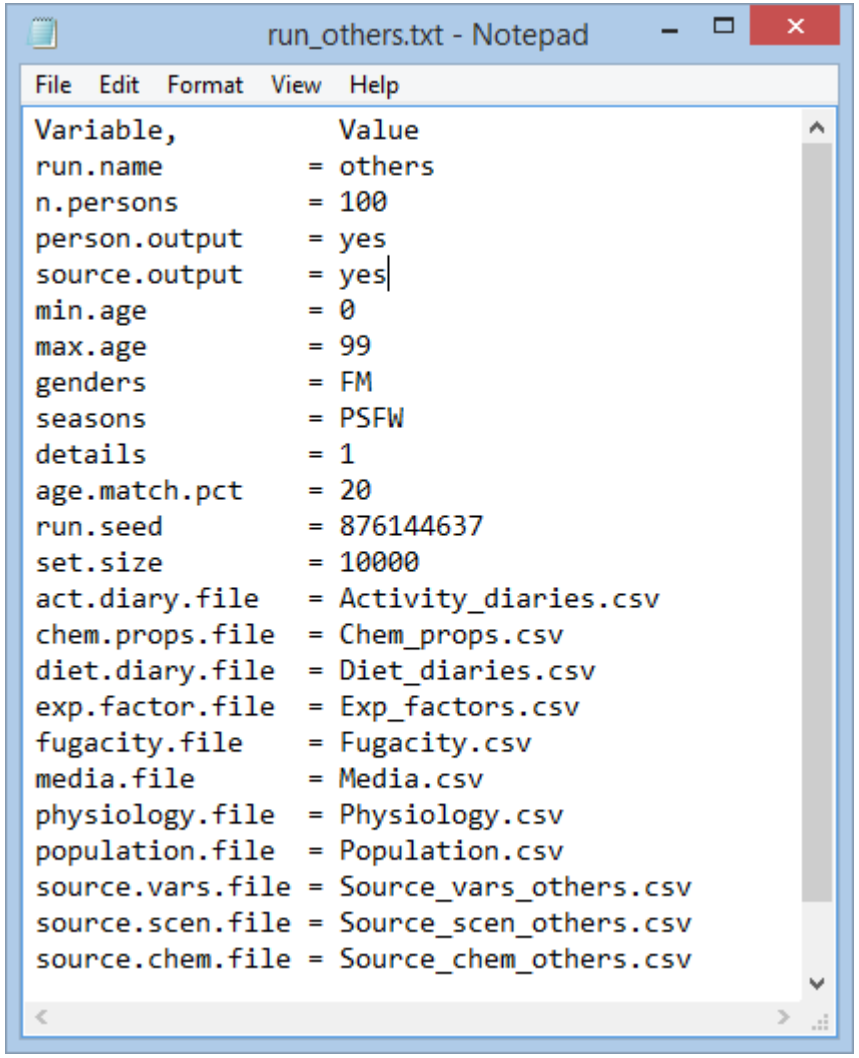
SHEDS Home Directory Structure

- We will cover set-up from R package in Demo



Output Files

Run File



- Text file
- Main control file for each run
- Controls:
  - General settings
  - Input files to be used for the run

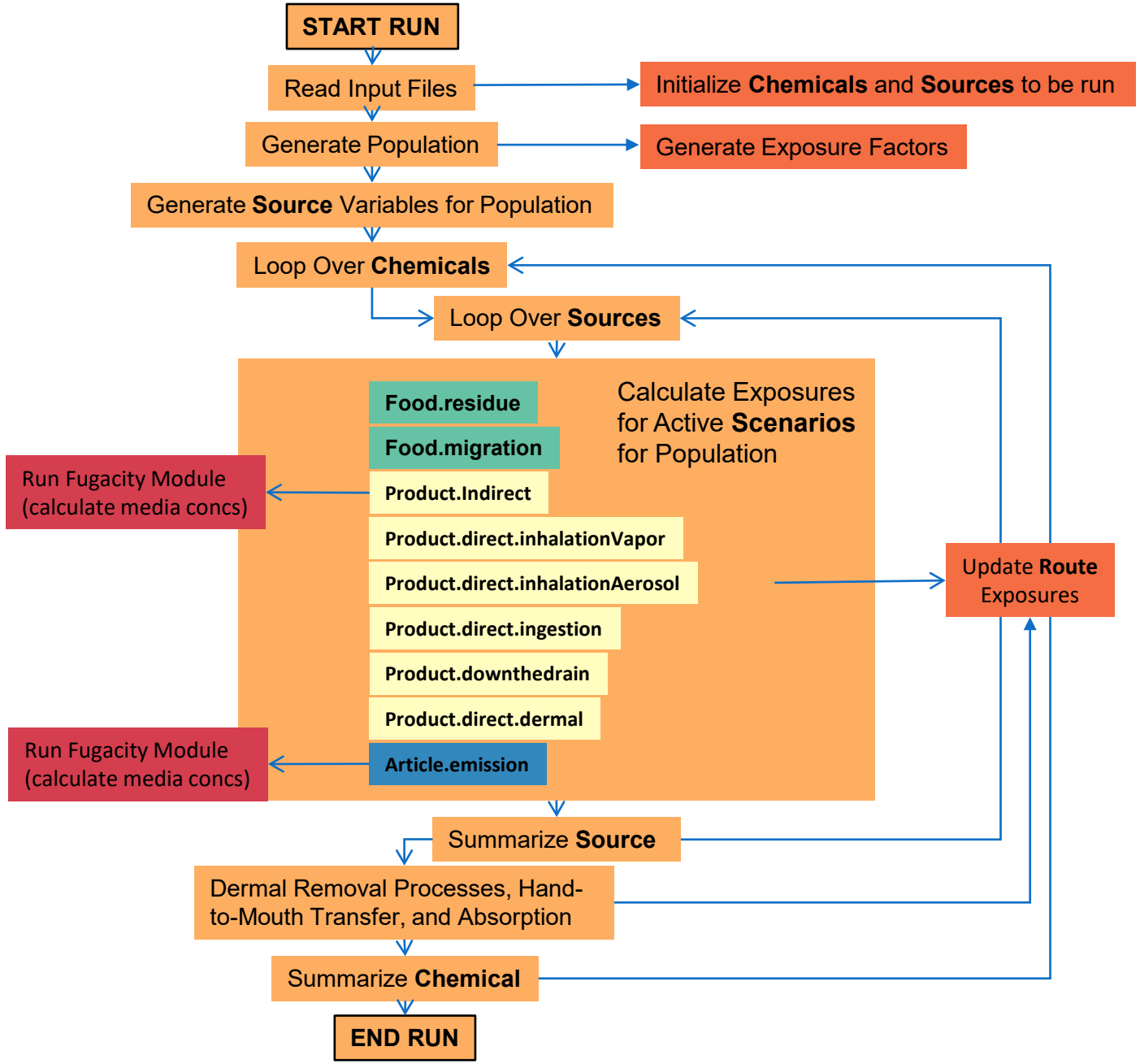
Model Run Overview

Run-Specific Input Files

- **Run File**
- **Source-Scenario File**
- **Source-Chemical File**
- **Source-Variable File**

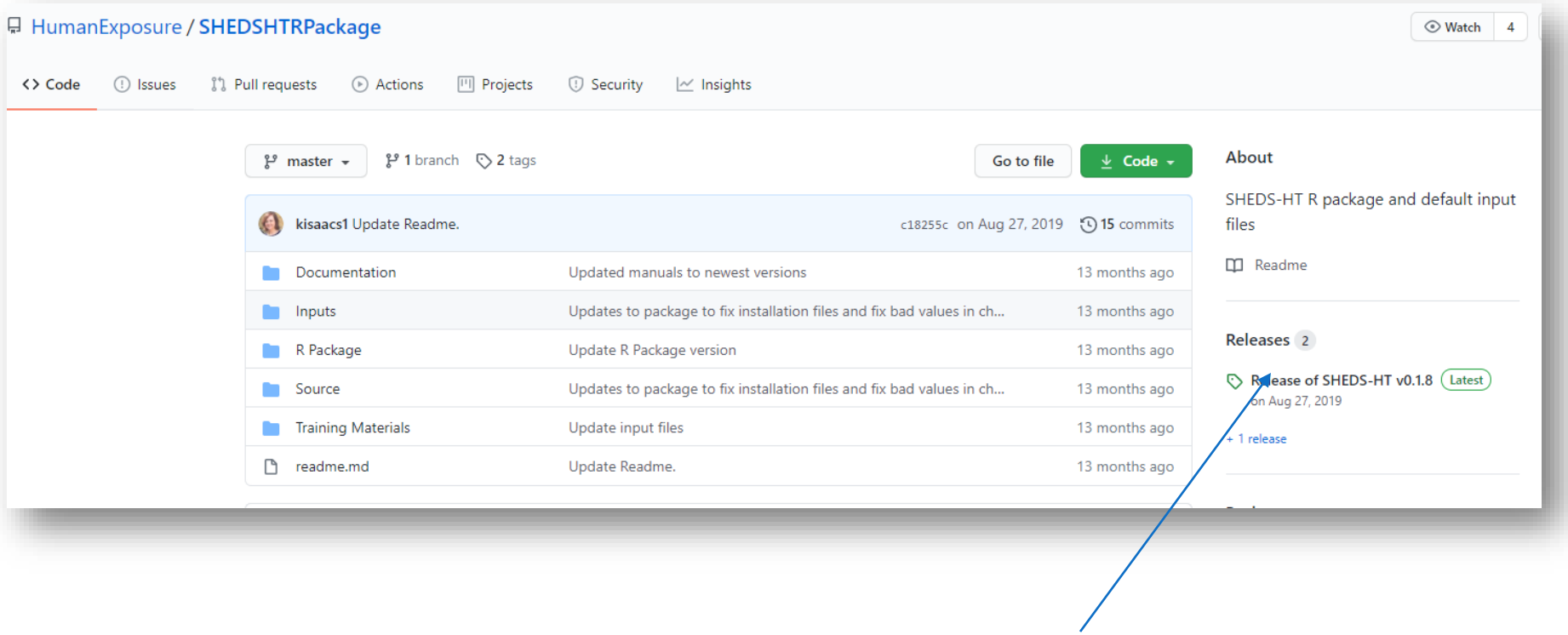
General Input Files

- **Activity Diary File**
- **Chemical Property File**
- **Dietary Diary File**
- **Exposure Factor File**
- **Fugacity File**
- **Media File**
- **Physiology File**
- **Population File**



Example: Running CPDat in SHEDS

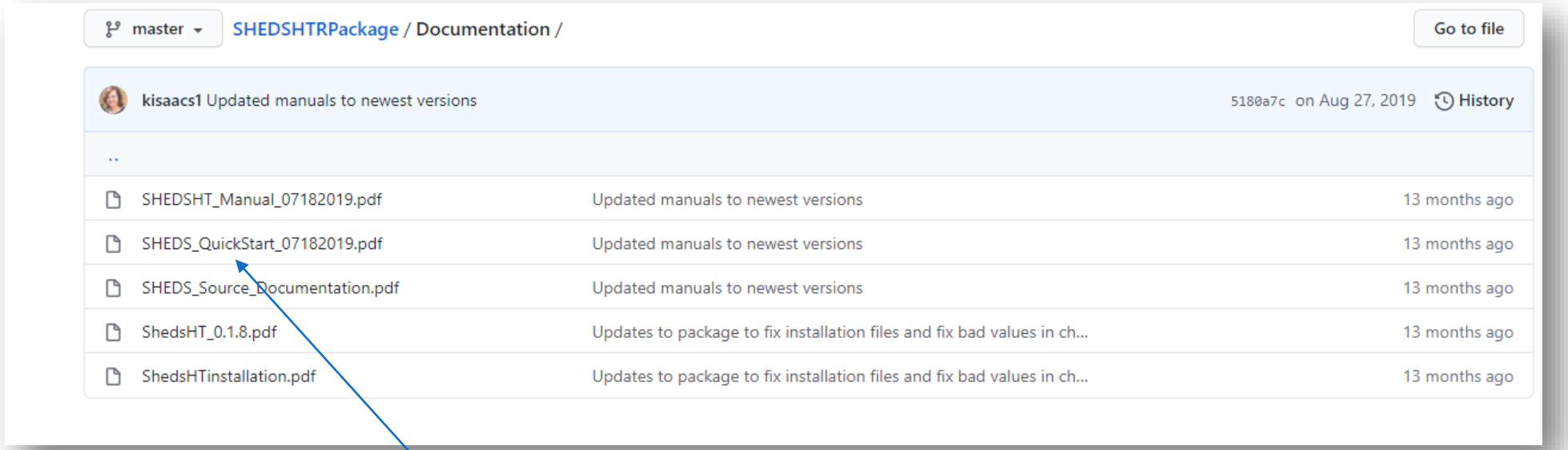
https://github.com/HumanExposure/SHEDSHTRPackage



Current release

Quick Start Guide

https://github.com/HumanExposure/SHEDSHTRPackage



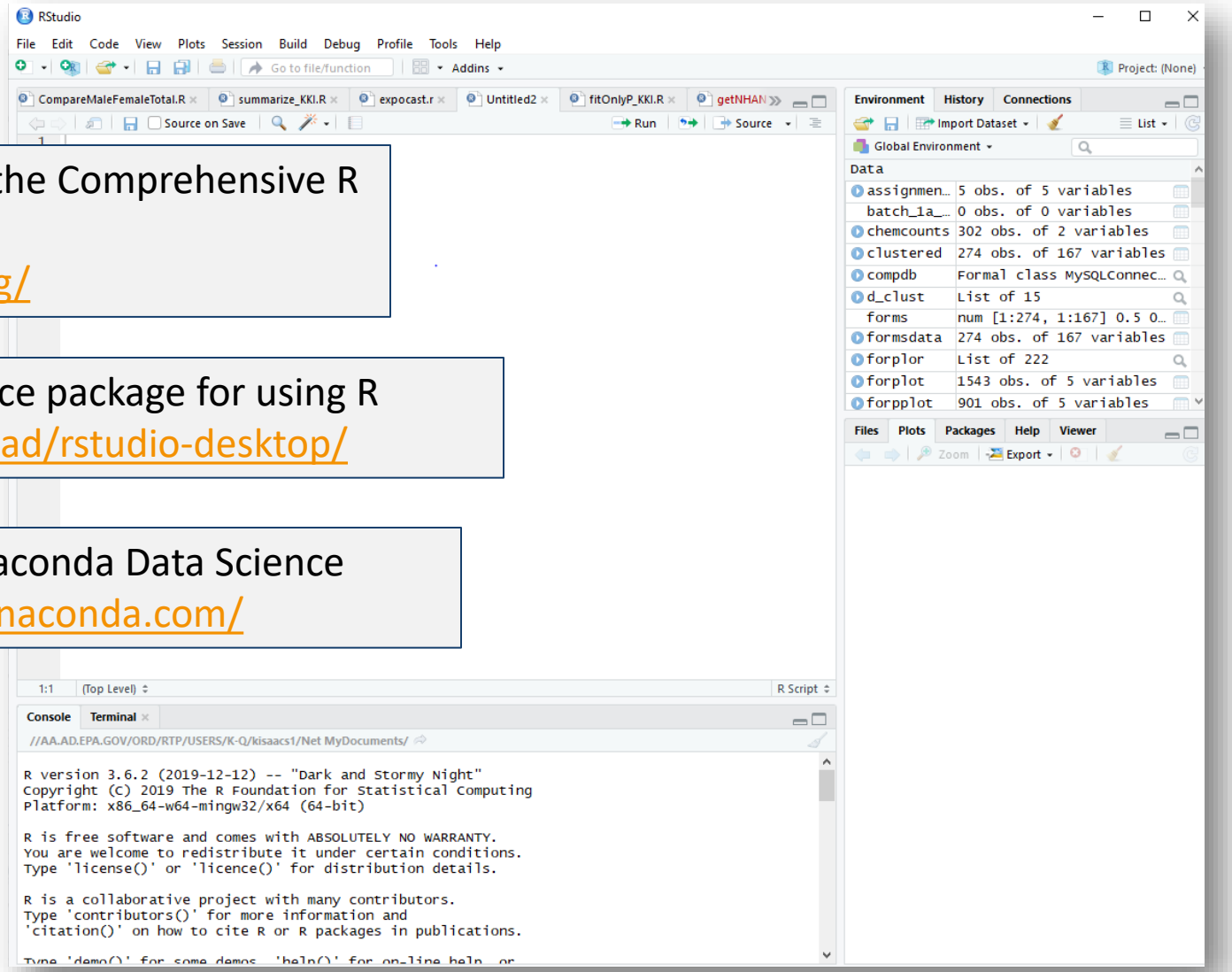
Quick Start Manual Provides step by step instructions for running all products in the 2017 version of CPDat

R and R Studio

R is freely available from the Comprehensive R Archive Network (CRAN): https://cloud.r-project.org/

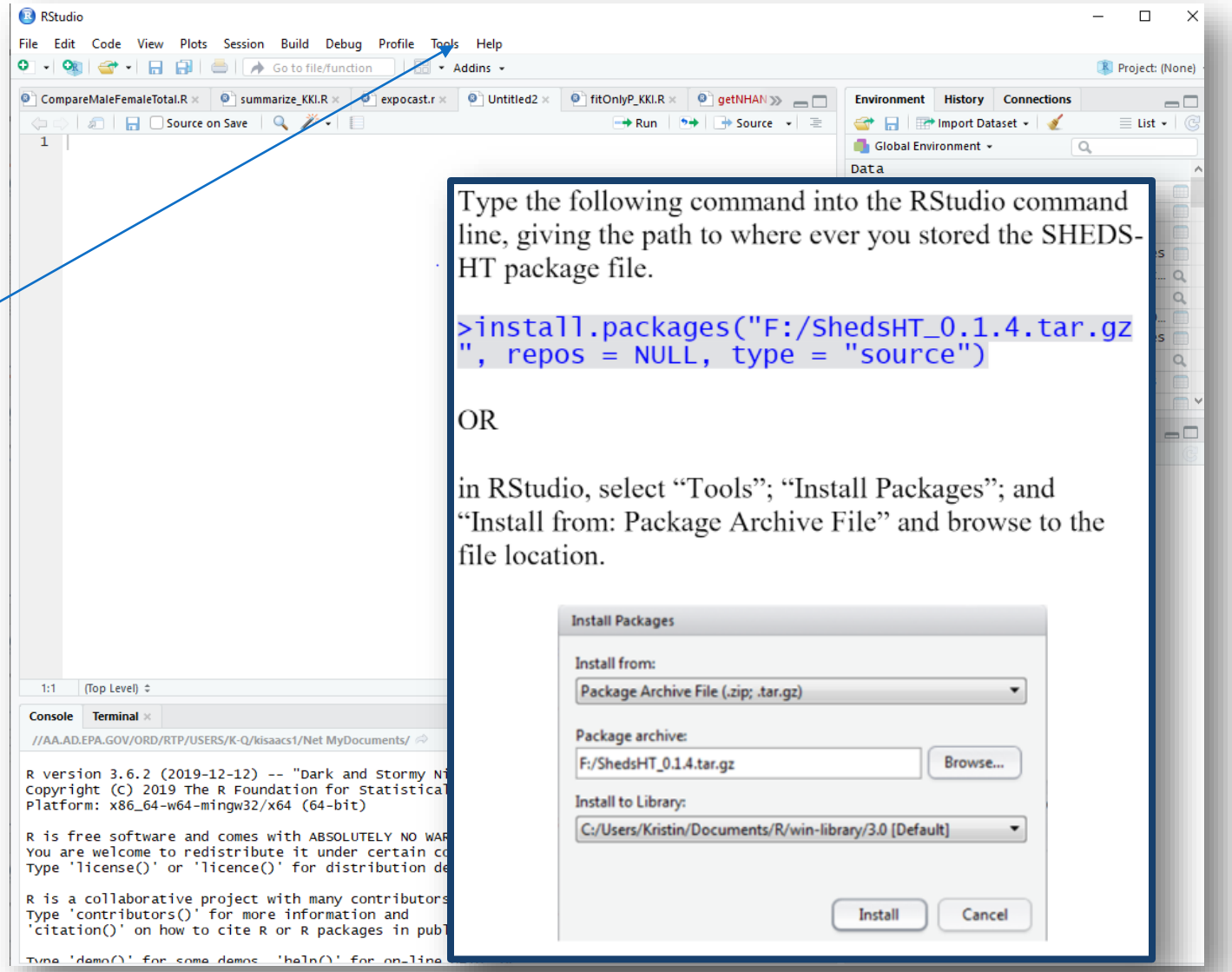
Rstudio: Free open source package for using R https://posit.co/download/rstudio-desktop/

Also available via the Anaconda Data Science Platform: https://www.anaconda.com/



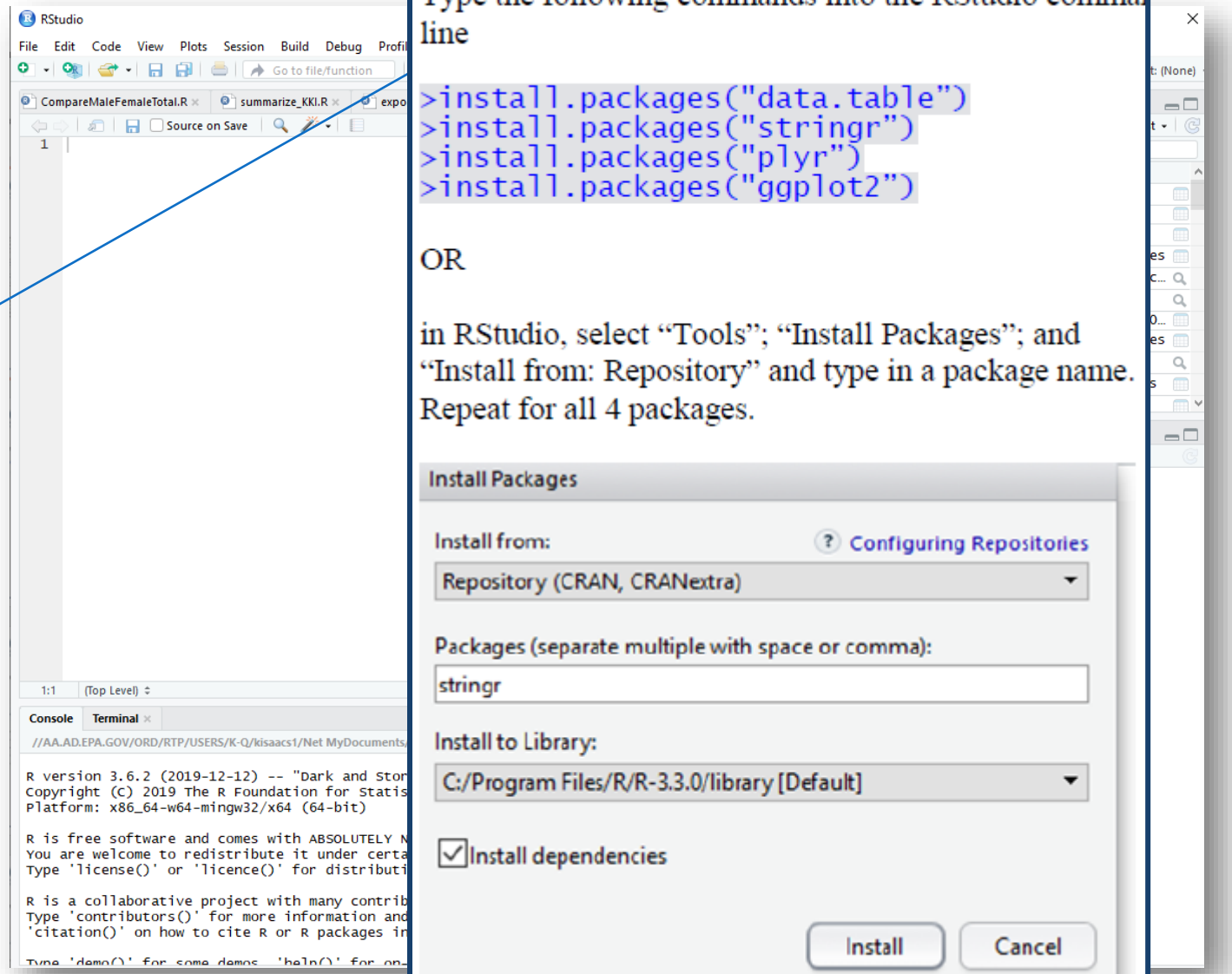
Installing SHEDS-HT

Tools



Installing Dependencies

Tools



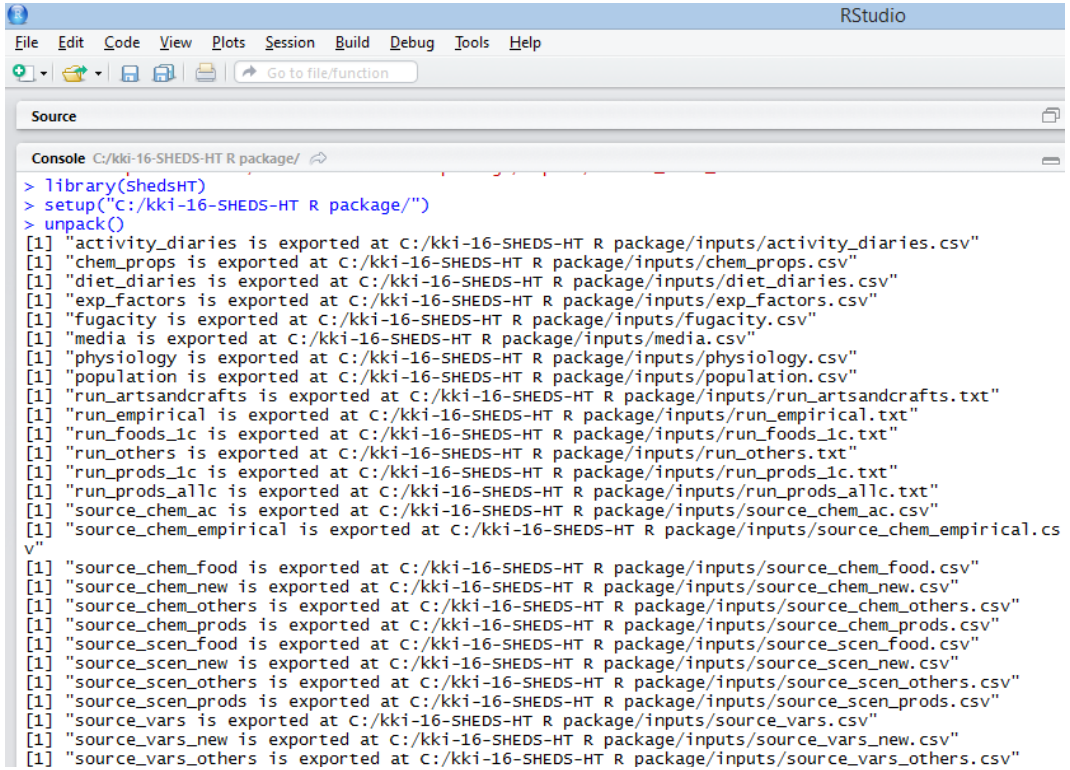
Type the following commands into the RStudio command line

```
>install.packages("data.table")
>install.packages("stringr")
>install.packages("plyr")
>install.packages("ggplot2")
```

OR

in RStudio, select "Tools"; "Install Packages"; and "Install from: Repository" and type in a package name. Repeat for all 4 packages.

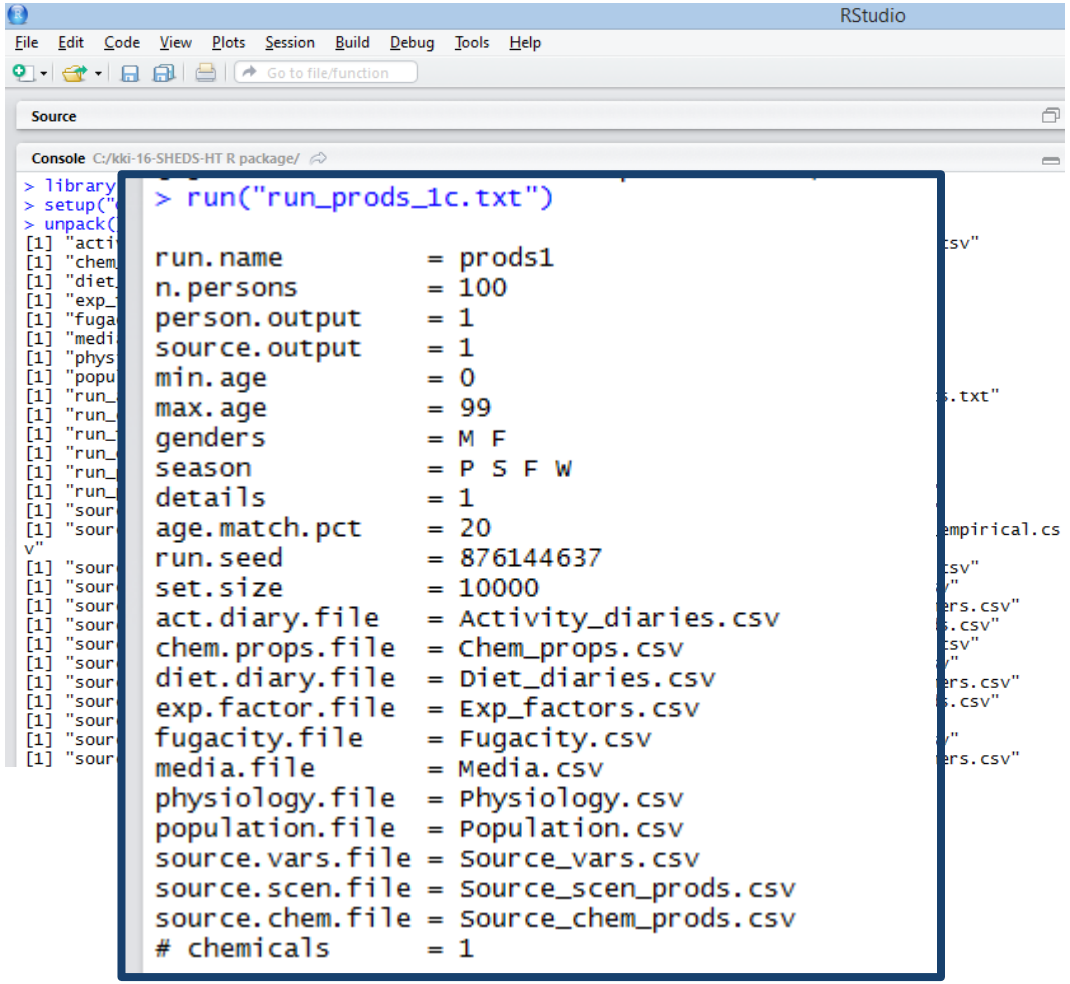
Performing a Run



- We will cover details in Demo

  - Install R Package and dependencies
  - Load R package: **>library(ShedsHT)**
  - Set up SHEDS-HT directory **>setup(path)**
  - Unpack input files **>unpack()**

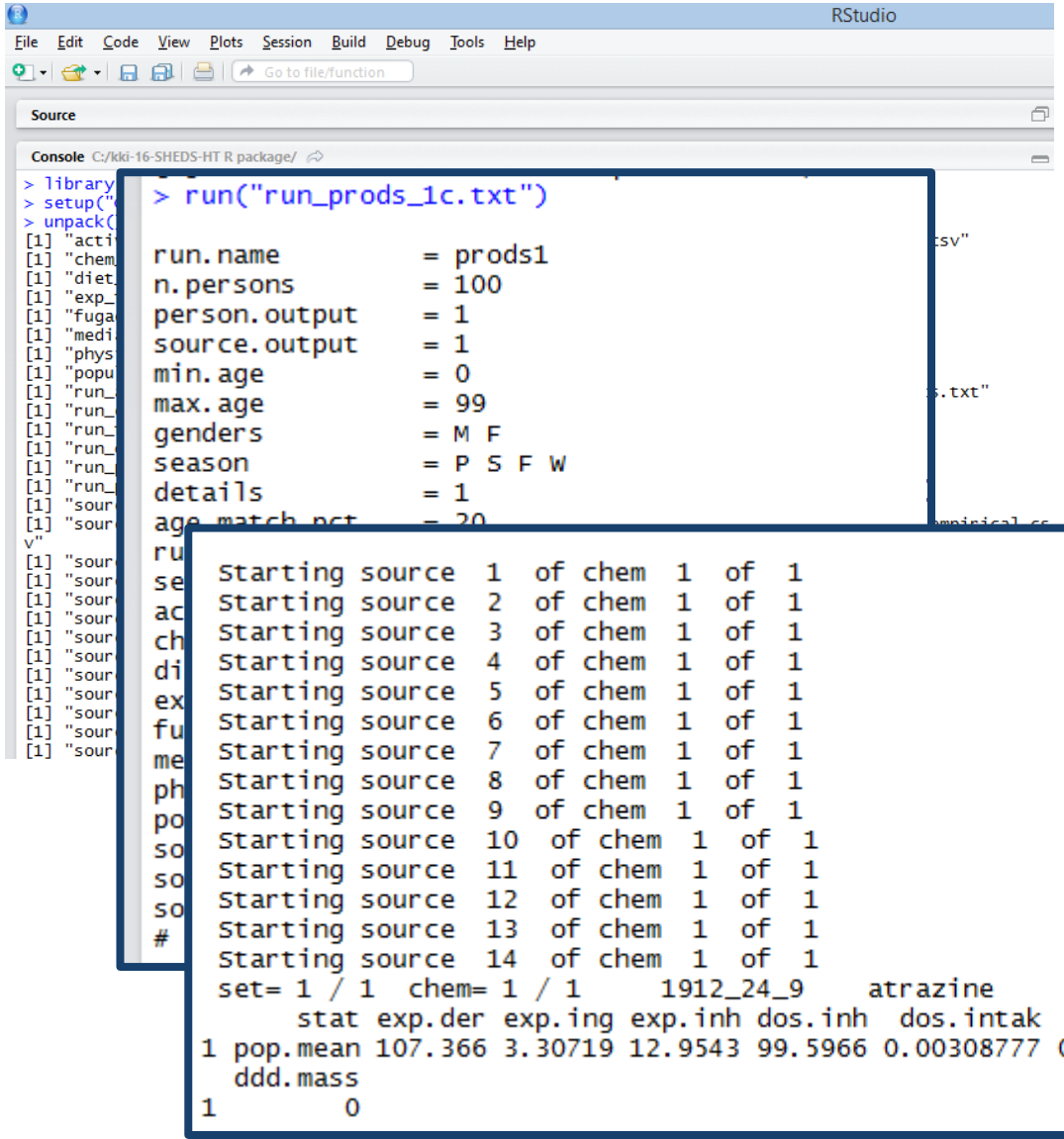
Performing a Run



- We will cover details in Demo

  - Install R Package and dependencies
  - Load R package: **>library(ShedsHT)**
  - Set up SHEDS-HT directory **>setup(path)**
  - Unpack input files **>unpack()**
  - Call run: **>run("runfile.txt")**

Performing a Run

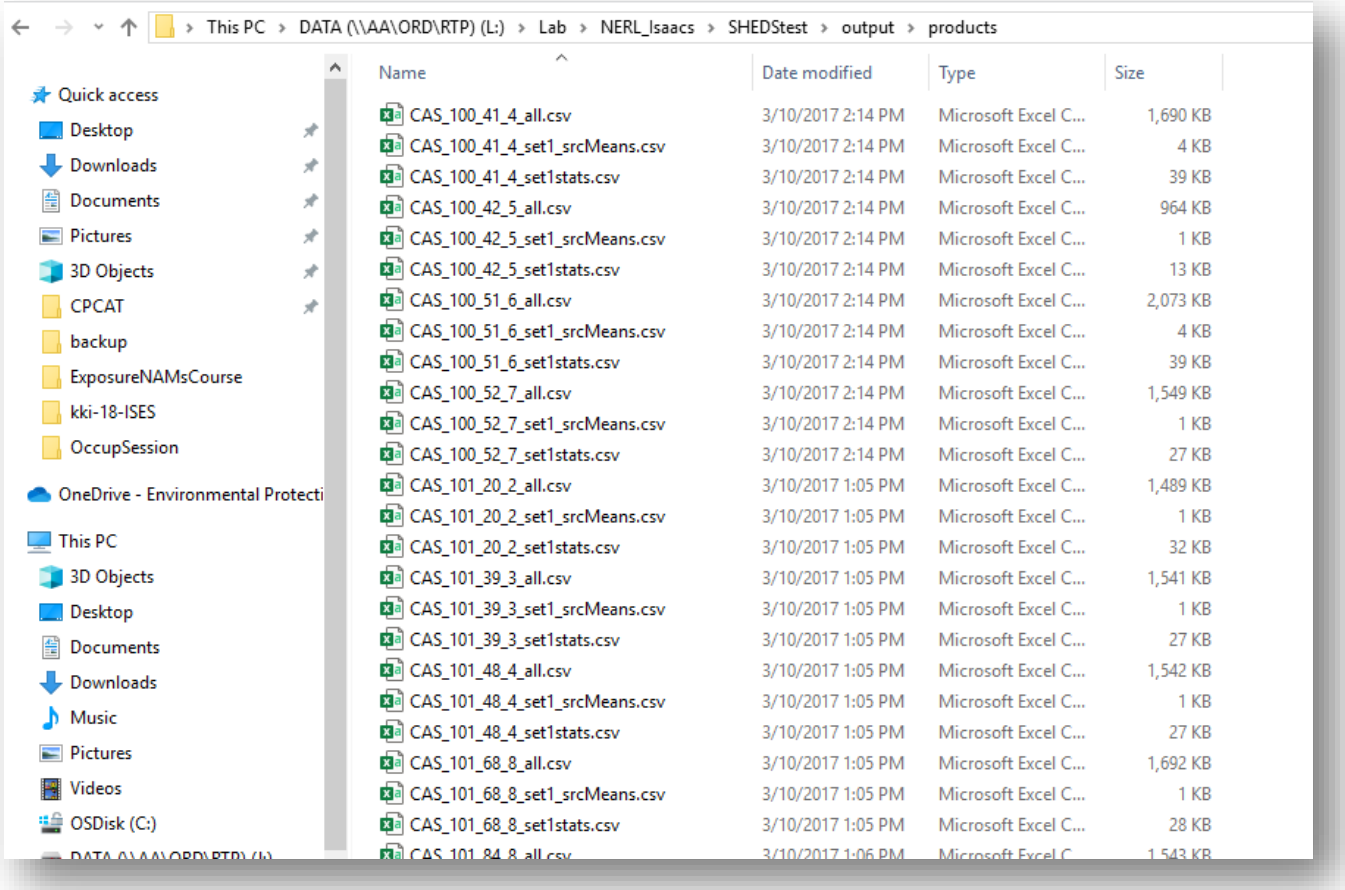


- We will cover details in Demo

- Install R Package and dependencies
- Load R package: **>library(ShedsHT)**
- Set up SHEDS-HT directory **>setup(path)**
- Unpack input files **>unpack()**
- Call run: **>run("runCPDat.txt")**

Output for Each Chemical in the Run in “Output” Folder

- SHEDS-HT also contains functions for combining select metrics for each chemical into a combined file (for data analyses and plotting)



Demonstration: Running CPDat V3 Consumer Product Sources in SHEDS-HT

Extra Slides: For Tool Mentoring Session, Questions, and Reference

Exposure Scenarios

Exposure Scenarios

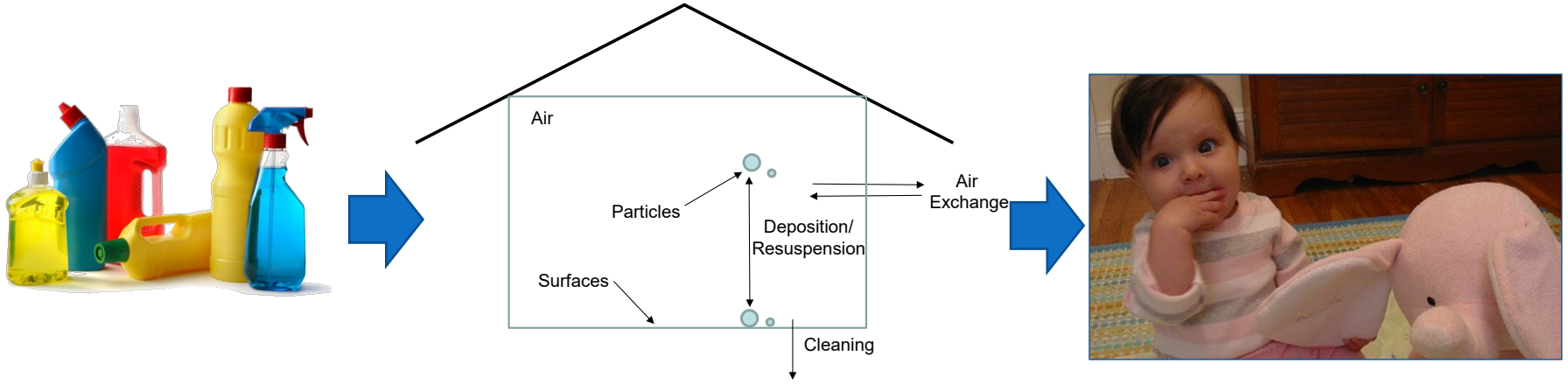
SHEDS Technical Manual Sections 4.6.3-4.6.6.

- **Product.Direct Scenarios**
  - Formulated similarly to other available models; probabilistic
  - Dependent on source-specific **frequency** of consumer product use, population **prevalence**, **mass** of product used, and product chemical **weight fraction (composition)**
  - Dermal: fraction retained on skin, fraction in contact with skin
  - Inhalation: aerosol mass or vapor: depends on Vp or fraction aerosolized
  - Ingestion: fraction ingested during use

Exposure Scenarios

SHEDS Technical Manual Sections 4.6.8 and 4.6.9.

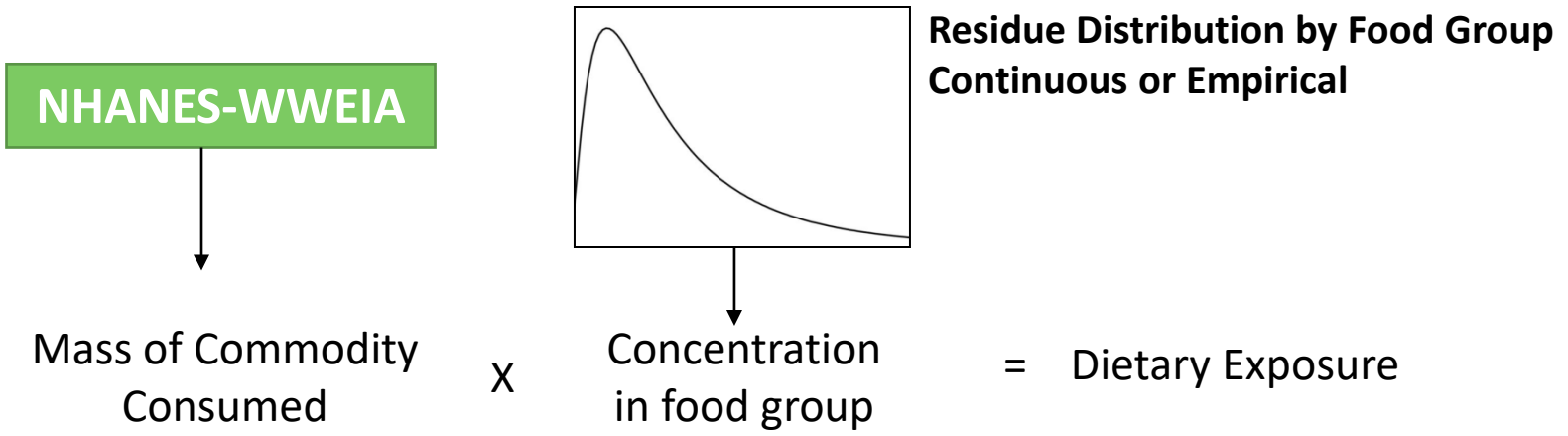
- **Product.Indirect and Article.Emission Scenarios**
  - Fugacity module is used to model the fate and transport of chemical within a home
  - Bolus application: media concentrations calculated for a sampled day from last application based on frequency of consumer product use
  - Constant emission: air concentrations due to area emission source based on steady-state air concentration at surface ($y_{0,}$ as in Little et al. 2013); other media concentrations via fugacity-based partitioning
  - Individuals breathe indoor air or touch contaminated surfaces post-use, resulting in exposure via inhalation, dermal, and ingestion (object-to-mouth, and hand-to-mouth) routes



Exposure Scenarios

SHEDS Technical Manual Section 4.6.1

- **Food.Residue Scenarios**
  - Consistent with SHEDS-MM dietary methods (by Xue et al.) reviewed during the 2010 FIFRA SAP
  - Consumption data: NHANES What We Eat In America (1999-2010)
  - Mapped to agricultural commodities using EPA Food Commodity Intake Database (FCID) recipe files
  - General SHED-HTS Dietary Input file is aggregated by by crop group
  - Other groups could be used
  - Aggregated to daily level – mass per food group

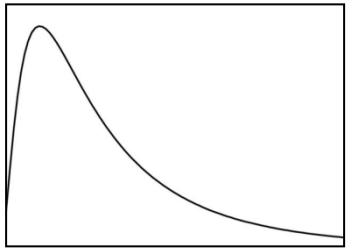


Exposure Scenarios

SHEDS Technical Manual Section 4.6.2

- **Food.Migration Scenario**
  - Similar to the Food.Residue scenario
  - SHEDS-HT does not currently contain methods for estimating migration but models can be run externally, and concentrations used (e.g., Biryol et al. *Environ. Intl.* 2017)
  - Concentrations distributions or empirical values must be provided
  - Two additional factors

NHANES-WWEIA

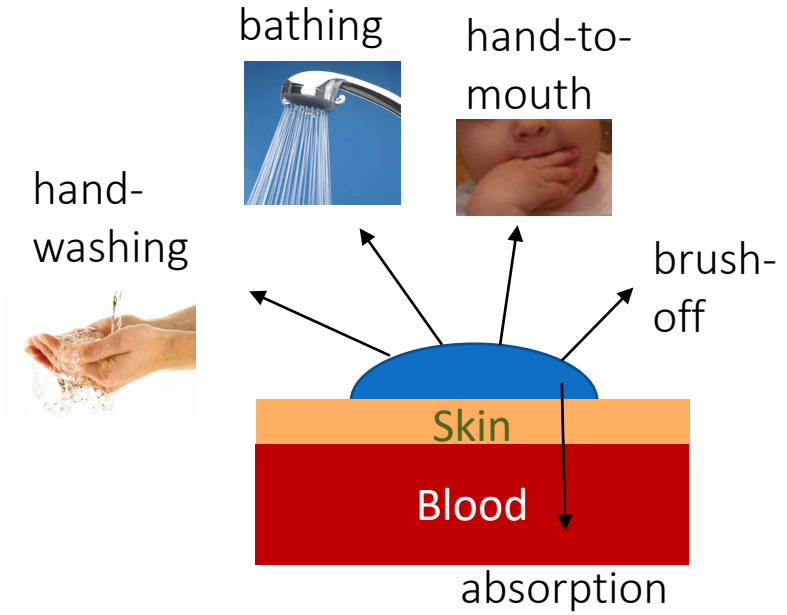


Mass of Commodity Consumed X Concentration in food group X Probability of Food Contact Substance Containing Chemical X Fraction of Food in Group Contacting FCS = Dietary Exposure

Dermal Removal Processes, Hand-to-Mouth Transfer, and Absorption by Route

- For each chemical, determining exposure contribution to each route from all sources/scenarios
- Apply dermal removal processes (bathing, hand washing, dermal absorption, brush-off, hand-to-mouth transfer) and calculate final dermal and ingestion exposures
- Apply route-specific absorption fractions and sum across routes to achieve total intake dose in mg/kg/bw-day

Five Competing Removal Processes for Dermal Exposure



SHEDS Technical Manual Sections 4.7 and 4.8

Product Source Categories

SHEDS-HT Default Product Sources

“P” for Product

SHEDS Technical Manual Tables B1-B3.

P

SHEDS-HT Default Product Sources

"P" for Product

Two-letter codes for general categories

Abbreviation	Description
AC	Arts and crafts
AP	Automotive products
HM	Home maintenance
HO	Home office
IH	Inside the home
LY	Lawn and yard
PC	Personal care
PE	Pesticides
PT	Pet-related products

SHEDS Technical Manual Tables B1-B3.

P.PC

SHEDS-HT Default Product Sources

"P" for Product

Two-letter codes for g

Abbreviation	Description
AC	Arts and crafts
AP	Automotive pro
HM	Home maintena
HO	Home office
IH	Inside the home
LY	Lawn and yard
PC	Personal care
PE	Pesticides
PT	Pet-related proc

Three digit codes for product types

Code	Description	Code	Description
P.AC.010	arts and crafts adhesive	P.LY.070	lawnmower fluids
P.AC.020	arts and crafts cleaner	P.LY.080	mulch
P.AC.030	arts and crafts finish	P.LY.090	pool chemicals
P.AC.040	arts and crafts paint	P.LY.100	potting soil
P.AC.050	body paint	P.LY.110	surface deicer
P.AC.060	bubble solution	P.LY.120	trees
P.AC.070	craft kit	P.PC.010	acne spot treatment
P.AC.080	crayons	P.PC.020	aftershave
P.AC.090	dye	P.PC.030	baby lotion
P.AC.100	fabric paints and sealers	P.PC.040	baby oil
P.AC.110	finger paint	P.PC.050	baby powder
P.AC.120	flocking	P.PC.060	baby shampoo
P.AC.130	fogger	P.PC.070	baby wash
P.AC.140	glaze	P.PC.080	baby wipes
P.AC.150	gun cleaner	P.PC.090	bar soap
P.AC.160	pens and markers	P.PC.100	bath oil
P.AC.170	play dough	P.PC.110	bath paints/crayons
P.AP.010	antifreeze	P.PC.120	bath salts
P.AP.020	auto air freshener	P.PC.130	bite relief

SHEDS Technical Manual Tables B1-B3.

P.PC.100

SHEDS-HT Default Product Sources

"P" for Product

Two-letter codes for g

Abbreviation	Description
AC	Arts and crafts
AP	Automotive pro
HM	Home maintena
HO	
IH	
LY	
PC	
PE	
PT	

Three-digit codes for product types

Code	Description	Code	Description
P.AC.010	arts and crafts adhesive	P.LY.070	lawnmower fluids
P.AC.020	arts and crafts cleaner	P.LY.080	mulch
P.AC.030	arts and crafts finish	P.LY.090	pool chemicals
P.AC.040	arts and crafts paint	P.LY.100	potting soil
P.AC.050	body paint	P.LY.110	surface deicer
P.AC.060	bubble solution	P.LY.120	trees
P.AC.070	craft kit	P.PC.010	acne spot treatment

Code	Description	Code	Description
001	acne	019	permanent
002	algaecide	020	pet
003	chlorinating	021	pet|spray
004	dandruff	022	ph control
005	exterior	023	powder
006	exterior|spray	024	professional
007	gel	025	shock
008	gel|spray	026	skin
009	interior	027	skin|spray
010	interior|spray	028	solid
011	leave-in	029	spray
012	leave-in|spray	030	temporary
013	liquid	031	temporary|spray
014	mousse	099	other
015	mousse|spray	100	children
016	oil or diffuse	101	children|spray
018	other|spray		

r

oo

crayons

Three-digit codes for refined product types

SHEDS Technical Manual Tables B1-B3.

P.PC.100.029

323 Product Sources (Categories)

SHEDS-HT Input Files

Source –Scenario File

SHEDS Technical Manual Section 3.3.10.

source.type	source.id	source.description	indoor	food. residue	food. migration	product. direct. dermal	product. direct. ingestion	product. direct. inhalationaerosol	product. direct. inhalationvapor	product. downthedrain	product. indirect	article. emission
Product	P.AC.010.029	arts and crafts adhesive-spray	1	0	0	1	0	1	1	0	1	0
Product	P.AC.010.099	arts and crafts adhesive-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.020.099	arts and crafts cleaner	1	0	0	1	0	0	1	0	1	0
Product	P.AC.030.029	arts and crafts finish-spray	1	0	0	1	0	1	1	0	0	0
Product	P.AC.030.099	arts and crafts finish-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.040.099	arts and crafts paint	1	0	0	1	0	0	1	0	1	0
Product	P.AC.050.029	body paint-spray	1	0	0	1	0	1	1	0	0	0
Product	P.AC.050.099	body paint-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.060.099	bubble solution	1	0	0	1	0	0	1	0	0	0
Product	P.AC.070.099	craft kit	1	0	0	1	0	0	1	0	0	0
Product	P.AC.080.099	crayons	1	0	0	1	1	0	1	0	0	0
Product	P.AC.090.099	dye	1	0	0	1	0	0	1	0	0	0
Product	P.AC.100.029	fabric paints and sealers-spray	1	0	0	1	0	1	1	0	1	0
Product	P.AC.100.099	fabric paints and sealers-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.110.099	finger paint	1	0	0	1	1	0	1	0	0	0
Product	P.AC.120.029	flocking	1	0	0	1	0	0	1	0	1	0
Product	P.AC.130.099	fogger	1	0	0	0	0	0	1	0	1	0
Product	P.AC.140.099	glaze	1	0	0	1	0	0	1	0	0	0
Product	P.AC.150.099	gun cleaner	1	0	0	1	0	0	1	0	0	0
Product	P.AC.160.099	pens and markers	1	0	0	1	1	0	1	0	0	0
Product	P.AC.170.017	play dough	1	0	0	1	1	0	1	0	0	0
Product	P.AP.010.099	antifreeze	1	0	0	1	0	0	1	0	0	0
Product	P.AP.020.029	auto air freshener-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.020.099	auto air freshener-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.030.029	auto fluids and additives-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.030.099	auto fluids and additives-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.040.029	auto lubricant-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.040.099	auto lubricant-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.050.029	auto paint-spray	0	0	0	1	0	1	1	0	0	0

Source –Scenario File

SHEDS Technical Manual Section 3.3.10.

Source Information

source.type	source.id	source.description	indoor	food. residue	food. migration	product. direct. dermal	product. direct. ingestion	product. direct. inhalationaerosol	product. direct. inhalationvapor	product. downthedrain	product. indirect	article. emission
Product	P.AC.010.029	arts and crafts adhesive-spray	1	0	0	1	0	1	1	0	1	0
Product	P.AC.010.099	arts and crafts adhesive-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.020.099	arts and crafts cleaner	1	0	0	1	0	0	1	0	1	0
Product	P.AC.030.029	arts and crafts finish-spray	1	0	0	1	0	1	1	0	0	0
Product	P.AC.030.099	arts and crafts finish-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.040.099	arts and crafts paint	1	0	0	1	0	0	1	0	1	0
Product	P.AC.050.029	body paint-spray	1	0	0	1	0	1	1	0	0	0
Product	P.AC.050.099	body paint-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.060.099	bubble solution	1	0	0	1	0	0	1	0	0	0
Product	P.AC.070.099	craft kit	1	0	0	1	0	0	1	0	0	0
Product	P.AC.080.099	crayons	1	0	0	1	1	0	1	0	0	0
Product	P.AC.090.099	dye	1	0	0	1	0	0	1	0	0	0
Product	P.AC.100.029	fabric paints and sealers-spray	1	0	0	1	0	1	1	0	1	0
Product	P.AC.100.099	fabric paints and sealers-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.110.099	finger paint	1	0	0	1	1	0	1	0	0	0
Product	P.AC.120.029	flocking	1	0	0	1	0	0	1	0	1	0
Product	P.AC.130.099	fogger	1	0	0	0	0	0	1	0	1	0
Product	P.AC.140.099	glaze	1	0	0	1	0	0	1	0	0	0
Product	P.AC.150.099	gun cleaner	1	0	0	1	0	0	1	0	0	0
Product	P.AC.160.099	pens and markers	1	0	0	1	1	0	1	0	0	0
Product	P.AC.170.017	play dough	1	0	0	1	1	0	1	0	0	0
Product	P.AP.010.099	antifreeze	1	0	0	1	0	0	1	0	0	0
Product	P.AP.020.029	auto air freshener-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.020.099	auto air freshener-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.030.029	auto fluids and additives-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.030.099	auto fluids and additives-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.040.029	auto lubricant-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.040.099	auto lubricant-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.050.029	auto paint-spray	0	0	0	1	0	1	1	0	0	0

Source –Scenario File

SHEDS Technical Manual Section 3.3.10.

1=scenario active for this source ID

Source Information

Scenarios

source.type	source.id	source.description	indoor	food. residue	food. migration	product. direct. dermal	product. direct. ingestion	product. direct. inhalationaerosol	product. direct. inhalationvapor	product. downthedrain	product. indirect	article. emission
Product	P.AC.010.029	arts and crafts adhesive-spray	1	0	0	1	0	1	1	0	1	0
Product	P.AC.010.099	arts and crafts adhesive-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.020.099	arts and crafts cleaner	1	0	0	1	0	0	1	0	1	0
Product	P.AC.030.029	arts and crafts finish-spray	1	0	0	1	0	1	1	0	0	0
Product	P.AC.030.099	arts and crafts finish-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.040.099	arts and crafts paint	1	0	0	1	0	0	1	0	1	0
Product	P.AC.050.029	body paint-spray	1	0	0	1	0	1	1	0	0	0
Product	P.AC.050.099	body paint-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.060.099	bubble solution	1	0	0	1	0	0	1	0	0	0
Product	P.AC.070.099	craft kit	1	0	0	1	0	0	1	0	0	0
Product	P.AC.080.099	crayons	1	0	0	1	1	0	1	0	0	0
Product	P.AC.090.099	dye	1	0	0	1	0	0	1	0	0	0
Product	P.AC.100.029	fabric paints and sealers-spray	1	0	0	1	0	1	1	0	1	0
Product	P.AC.100.099	fabric paints and sealers-other	1	0	0	1	0	0	1	0	0	0
Product	P.AC.110.099	finger paint	1	0	0	1	1	0	1	0	0	0
Product	P.AC.120.029	flocking	1	0	0	1	0	0	1	0	1	0
Product	P.AC.130.099	fogger	1	0	0	0	0	0	1	0	1	0
Product	P.AC.140.099	glaze	1	0	0	1	0	0	1	0	0	0
Product	P.AC.150.099	gun cleaner	1	0	0	1	0	0	1	0	0	0
Product	P.AC.160.099	pens and markers	1	0	0	1	1	0	1	0	0	0
Product	P.AC.170.017	play dough	1	0	0	1	1	0	1	0	0	0
Product	P.AP.010.099	antifreeze	1	0	0	1	0	0	1	0	0	0
Product	P.AP.020.029	auto air freshener-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.020.099	auto air freshener-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.030.029	auto fluids and additives-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.030.099	auto fluids and additives-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.040.029	auto lubricant-spray	0	0	0	1	0	1	1	0	0	0
Product	P.AP.040.099	auto lubricant-other	0	0	0	1	0	0	1	0	0	0
Product	P.AP.050.029	auto paint-spray	0	0	0	1	0	1	1	0	0	0

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Source–Variable File

SHEDS Technical Manual Section 3.3.12.

source.type	source.id	source.description	variable	units	gender	min.age	max.age	form	mean	CV
Product	P.AC.010.029	**arts and crafts** adhesive-other	duration	minutes	B	0	99	Lognormal	10	1
Product	P.AC.010.029	arts and crafts adhesive-other	f.aerosol	[-]	B	0	99	POINT	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	f.contact	[-]	B	0	99	Point	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	f.ingested	[-]	B	0	99	Lognormal	0.005	0.2
Product	P.AC.010.029	arts and crafts adhesive-other	f.residual	[-]	B	0	99	Point	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	mass	g	B	0	99	Lognormal	255	1
Product	P.AC.010.029	arts and crafts adhesive-other	use.freq	1/year	B	0	99	lognormal	12	1
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	B	0	12	point	0.05	0
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	M	13	99	point	0.4	0
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	W	13	99	point	0.4	0
Product	P.AC.010.029	arts and crafts adhesive-other	volume	m3	B	0	99	normal	48	0.5

Source–Variable File

SHEDS Technical Manual Section 3.3.12.

Source Information

source.type	source.id	source.description	variable	units	gender	min.age	max.age	form	mean	CV
Product	P.AC.010.029	**arts and crafts** adhesive-other	duration	minutes	B	0	99	Lognormal	10	1
Product	P.AC.010.029	arts and crafts adhesive-other	f.aerosol	[-]	B	0	99	POINT	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	f.contact	[-]	B	0	99	Point	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	f.ingested	[-]	B	0	99	Lognormal	0.005	0.2
Product	P.AC.010.029	arts and crafts adhesive-other	f.residual	[-]	B	0	99	Point	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	mass	g	B	0	99	Lognormal	255	1
Product	P.AC.010.029	arts and crafts adhesive-other	use.freq	1/year	B	0	99	lognormal	12	1
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	B	0	12	point	0.05	0
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	M	13	99	point	0.4	0
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	W	13	99	point	0.4	0
Product	P.AC.010.029	arts and crafts adhesive-other	volume	m3	B	0	99	normal	48	0.5

Source–Variable File

SHEDS Technical Manual Section 3.3.12.

Source Information

Source-specific variables*

source.type	source.id	source.description	variable	units	gender	min.age	max.age	form	mean	CV
Product	P.AC.010.029	**arts and crafts** adhesive-other	duration	minutes	B	0	99	Lognormal	10	1
Product	P.AC.010.029	arts and crafts adhesive-other	f.aerosol	[-]	B	0	99	POINT	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	f.contact	[-]	B	0	99	Point	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	f.ingested	[-]	B	0	99	Lognormal	0.005	0.2
Product	P.AC.010.029	arts and crafts adhesive-other	f.residual	[-]	B	0	99	Point	0.01	0
Product	P.AC.010.029	arts and crafts adhesive-other	mass	g	B	0	99	Lognormal	255	1
Product	P.AC.010.029	arts and crafts adhesive-other	use.freq	1/year	B	0	99	lognormal	12	1
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	B	0	12	point	0.05	0
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	M	13	99	point	0.4	0
Product	P.AC.010.029	arts and crafts adhesive-other	use.prev	[-]	W	13	99	point	0.4	0
Product	P.AC.010.029	arts and crafts adhesive-other	volume	m3	B	0	99	normal	48	0.5

**SHEDS will write error if a scenario is missing a required variable*

Source–Chemical File

SHEDS Technical Manual Section 3.3.11.

source.type	source.id	source.description	cas	variable	units	gender	min.age	max.age	form	mean	CV	value
Product	P.AC.010.029	arts and crafts adhesive-spray	67-64-1	f.chemical	[-]	B	0	99	empirical			0.2, 0.275, 0.2, 0.62, 0.75
Product	P.AC.010.099	arts and crafts adhesive-other	67-64-1	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	109-66-0	f.chemical	[-]	B	0	99	empirical			0.2
Product	P.AC.010.099	arts and crafts adhesive-other	109-66-0	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	110-54-3	f.chemical	[-]	B	0	99	empirical			0.075, 0.225, 0.0055, 0.35
Product	P.AC.010.099	arts and crafts adhesive-other	110-54-3	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	106-97-8	f.chemical	[-]	B	0	99	empirical			0.175, 0.12
Product	P.AC.010.099	arts and crafts adhesive-other	106-97-8	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	115-10-6	f.chemical	[-]	B	0	99	empirical			0.1, 0.425, 0.2
Product	P.AC.010.099	arts and crafts adhesive-other	115-10-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	74-98-6	f.chemical	[-]	B	0	99	empirical			0.1, 0.13
Product	P.AC.010.099	arts and crafts adhesive-other	74-98-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-28-5	f.chemical	[-]	B	0	99	empirical			0.1
Product	P.AC.010.099	arts and crafts adhesive-other	75-28-5	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-83-2	f.chemical	[-]	B	0	99	empirical			0.03
Product	P.AC.010.099	arts and crafts adhesive-other	75-83-2	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	79-29-8	f.chemical	[-]	B	0	99	empirical			0.05
Product	P.AC.010.099	arts and crafts adhesive-other	79-29-8	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	107-83-5	f.chemical	[-]	B	0	99	empirical			0.15
Product	P.AC.010.099	arts and crafts adhesive-other	107-83-5	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	110-82-7	f.chemical	[-]	B	0	99	empirical			0.15, 0.095
Product	P.AC.010.099	arts and crafts adhesive-other	110-82-7	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-37-6	f.chemical	[-]	B	0	99	empirical			0.03
Product	P.AC.010.099	arts and crafts adhesive-other	75-37-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	79-20-9	f.chemical	[-]	B	0	99	empirical			0.275
Product	P.AC.010.099	arts and crafts adhesive-other	79-20-9	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	84-74-2	f.chemical	[-]	B	0	99	empirical			0.035
Product	P.AC.010.099	arts and crafts adhesive-other	84-74-2	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	1336-21-6	f.chemical	[-]	B	0	99	empirical			1.00E-04

Source–Chemical File

SHEDS Technical Manual Section 3.3.11.

Source Information

source.type	source.id	source.description	cas	variable	units	gender	min.age	max.age	form	mean	CV	value
Product	P.AC.010.029	arts and crafts adhesive-spray	67-64-1	f.chemical	[-]	B	0	99	empirical			0.2, 0.275, 0.2, 0.62, 0.75
Product	P.AC.010.099	arts and crafts adhesive-other	67-64-1	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	109-66-0	f.chemical	[-]	B	0	99	empirical			0.2
Product	P.AC.010.099	arts and crafts adhesive-other	109-66-0	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	110-54-3	f.chemical	[-]	B	0	99	empirical			0.075, 0.225, 0.0055, 0.35
Product	P.AC.010.099	arts and crafts adhesive-other	110-54-3	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	106-97-8	f.chemical	[-]	B	0	99	empirical			0.175, 0.12
Product	P.AC.010.099	arts and crafts adhesive-other	106-97-8	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	115-10-6	f.chemical	[-]	B	0	99	empirical			0.1, 0.425, 0.2
Product	P.AC.010.099	arts and crafts adhesive-other	115-10-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	74-98-6	f.chemical	[-]	B	0	99	empirical			0.1, 0.13
Product	P.AC.010.099	arts and crafts adhesive-other	74-98-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-28-5	f.chemical	[-]	B	0	99	empirical			0.1
Product	P.AC.010.099	arts and crafts adhesive-other	75-28-5	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-83-2	f.chemical	[-]	B	0	99	empirical			0.03
Product	P.AC.010.099	arts and crafts adhesive-other	75-83-2	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	79-29-8	f.chemical	[-]	B	0	99	empirical			0.05
Product	P.AC.010.099	arts and crafts adhesive-other	79-29-8	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	107-83-5	f.chemical	[-]	B	0	99	empirical			0.15
Product	P.AC.010.099	arts and crafts adhesive-other	107-83-5	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	110-82-7	f.chemical	[-]	B	0	99	empirical			0.15, 0.095
Product	P.AC.010.099	arts and crafts adhesive-other	110-82-7	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-37-6	f.chemical	[-]	B	0	99	empirical			0.03
Product	P.AC.010.099	arts and crafts adhesive-other	75-37-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	79-20-9	f.chemical	[-]	B	0	99	empirical			0.275
Product	P.AC.010.099	arts and crafts adhesive-other	79-20-9	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	84-74-2	f.chemical	[-]	B	0	99	empirical			0.035
Product	P.AC.010.099	arts and crafts adhesive-other	84-74-2	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	1336-21-6	f.chemical	[-]	B	0	99	empirical			1.00E-04

Source–Chemical File

SHEDS Technical Manual Section 3.3.11.

Source Information

Chemical

*Chemical-Specific Variables Parameters

(here weight fraction and chemical prevalence)

source.type	source.id	source.description	cas	variable	units	gender	min.age	max.age	form	mean	CV	value
Product	P.AC.010.029	arts and crafts adhesive-spray	67-64-1	f.chemical	[-]	B	0	99	empirical			0.2, 0.275, 0.2, 0.62, 0.75
Product	P.AC.010.099	arts and crafts adhesive-other	67-64-1	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	109-66-0	f.chemical	[-]	B	0	99	empirical			0.2
Product	P.AC.010.099	arts and crafts adhesive-other	109-66-0	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	110-54-3	f.chemical	[-]	B	0	99	empirical			0.075, 0.225, 0.0055, 0.35
Product	P.AC.010.099	arts and crafts adhesive-other	110-54-3	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	106-97-8	f.chemical	[-]	B	0	99	empirical			0.175, 0.12
Product	P.AC.010.099	arts and crafts adhesive-other	106-97-8	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	115-10-6	f.chemical	[-]	B	0	99	empirical			0.1, 0.425, 0.2
Product	P.AC.010.099	arts and crafts adhesive-other	115-10-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	74-98-6	f.chemical	[-]	B	0	99	empirical			0.1, 0.13
Product	P.AC.010.099	arts and crafts adhesive-other	74-98-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-28-5	f.chemical	[-]	B	0	99	empirical			0.1
Product	P.AC.010.099	arts and crafts adhesive-other	75-28-5	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-83-2	f.chemical	[-]	B	0	99	empirical			0.03
Product	P.AC.010.099	arts and crafts adhesive-other	75-83-2	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	79-29-8	f.chemical	[-]	B	0	99	empirical			0.05
Product	P.AC.010.099	arts and crafts adhesive-other	79-29-8	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	107-83-5	f.chemical	[-]	B	0	99	empirical			0.15
Product	P.AC.010.099	arts and crafts adhesive-other	107-83-5	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	110-82-7	f.chemical	[-]	B	0	99	empirical			0.15, 0.095
Product	P.AC.010.099	arts and crafts adhesive-other	110-82-7	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	75-37-6	f.chemical	[-]	B	0	99	empirical			0.03
Product	P.AC.010.099	arts and crafts adhesive-other	75-37-6	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	79-20-9	f.chemical	[-]	B	0	99	empirical			0.275
Product	P.AC.010.099	arts and crafts adhesive-other	79-20-9	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	84-74-2	f.chemical	[-]	B	0	99	empirical			0.035
Product	P.AC.010.099	arts and crafts adhesive-other	84-74-2	chem.prev	[-]	B	0	99	point	1	0	
Product	P.AC.010.099	arts and crafts adhesive-other	1336-21-6	f.chemical	[-]	B	0	99	empirical			1.00E-04

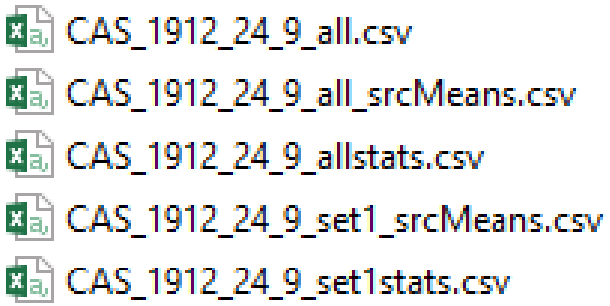
**SHEDS-HT will ignore chemical if missing a required variable*

SHEDS-HT Output Files

SHEDS Output Files

SHEDS Technical Manual Section 3.4.

- Created in new folder in “Outputs” directory with the same name as the Run
- Comma-separated value (CSV) files
- Each output file is chemical-specific, each file name is appended with chemical name (usually CASRN)
- For large number of individuals, SHEDS-HT runs multiple “sets” for optimizing speed. Some files are written for each set and are combined at the end of the run and given an “_all” extension.
- Three types of output files: All Individuals, Source Means, and Statistics



The All Individuals Output File

Exposure and dose metrics for every simulated individual for the chemical

person	gender	age	season	weekend	weight	exp.dermal	exp.inhal	exp.ingest	exp.diet	exp.nondiet	exp.drain	dose.inhal.ug	dose.intake.ug
1	M	27	W	0	59.978	13.997694	3.70E-05	2.209967	2.206132	0.003834	0	0.000326	2.245938
2	F	49	S	0	60.762	39.041696	1.90E-05	9.543337	9.535331	0.008006	0	0.000129	9.720123
3	M	82	F	0	73.557	31.368195	3.50E-05	1.917896	1.908342	0.009555	0	0.000385	2.187723
4	M	27	S	0	64.137	6.251821	3.60E-05	5.281458	5.267977	0.013481	0	0.000585	6.376272
5	F	3	W	0	11.494	18.67317	0.000247	0.650194	0.646349	0.003845	0	0.00109	1.171068
6	F	8	W	1	36.541	2.097236	3.00E-06	1.99112	1.990663	0.000456	0	2.30E-05	1.995508
7	F	26	F	0	58.193	2.77622	190.532886	3.11104	3.107556	0.003484	0	1644.496244	1647.687556
8	M	44	S	0	78.919	1.865448	3.00E-06	10.161121	10.160631	0.00049	0	2.30E-05	10.171563
9	M	6	F	0	19.178	127.206916	0.000325	2.055727	2.041036	0.014691	0	0.001536	2.1637
10	M	55	S	0	63.649	3.204044	2.70E-05	4.135855	4.128242	0.007613	0	0.000219	4.170739
11	F	35	W	0	74.231	17.943817	9.10E-05	3.341104	3.337106	0.003998	0	0.000908	4.448542
12	F	14	W	0	60.388	20.240516	0.000606	1.626264	1.623074	0.00319	0	0.005205	1.721052
13	F	73	F	1	47.865	950.967297	0.000954	4.446386	4.312327	0.134059	0	0.005691	5.553571
14	F	50	W	0	78.54	84.744533	0.000119	10.526335	10.245204	0.281132	0	9.00E-04	15.267697
15	M	5	P	1	20.599	47.00058	0.000138	1.406597	1.400411	0.006186	0	0.000632	2.859534
16	F	25	F	1	86.846	173.142736	9.40E-05	1.706744	1.681565	0.025179	0	0.000969	3.429888
17	F	57	W	1	48.446	0	0	0.951564	0.951564	0	0	0	0.951564
18	F	65	W	1	71.821	134.414926	0.001673	4.523777	4.259355	0.264422	0	0.011434	13.970333
19	M	12	S	0	46.86	28.391711	8.00E-05	2.646979	2.64035	0.006629	0	0.000584	2.667647
20	M	83	W	0	52.445	41.438019	2.30E-05	6.103663	6.095196	0.008467	0	0.000121	6.151268
21	M	69	S	0	75.314	7.354863	2.008075	7.868345	7.866734	0.001611	0	20.742349	28.624401
22	M	3	W	0	18.891	0	0	2.298012	2.298012	0	0	0	2.298012
23	M	5	F	1	22.493	161.909096	6.60E-05	1.662527	1.622322	0.040204	0	0.000346	3.982709

SHEDS Technical Manual Section 3.4.1.

The Statistics Output File

Population statistics by cohort (Total, M>F, age groups, women of childbearing age) for select exposure/dose metrics

		exp.dermal	exp.ingest	exp.inhal	dose.inhal	dose.intake	abs.dermal.ug	abs.ingest.ug	abs.inhal.ug	abs.tot.ug	abs.tot.mgkg	ddd.mass
Statistic	Cohort	ug/day	ug/day	ug/m3	ug/day	mg/kg/day	ug/day	ug/day	ug/day	ug/day	mg/kg/day	g/day
0.50%	Total	0	0.45274	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0
1%	Total	0	0.45274	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0
2.50%	Total	0	0.518785	0	0	1.53E-05	0	0.353257	0	0.355344	7.44E-06	0
5%	Total	0	0.71579	0	0	1.96E-05	0	0.439642	0	0.443794	1.14E-05	0
10%	Total	0	0.951564	2.00E-06	1.00E-05	2.41E-05	0	0.726728	2.00E-06	0.76502	1.32E-05	0
15%	Total	2.097236	1.225137	1.00E-05	7.00E-05	2.62E-05	0.000189	0.870716	1.10E-05	0.894217	1.47E-05	0
20%	Total	3.605379	1.626264	1.90E-05	0.000129	2.97E-05	0.000556	1.093802	2.10E-05	1.144045	1.69E-05	0
25%	Total	6.147302	1.735642	2.70E-05	0.000175	3.30E-05	0.000744	1.325966	2.80E-05	1.384025	2.16E-05	0
30%	Total	9.721634	1.925034	2.90E-05	0.000218	3.88E-05	0.001228	1.464601	3.50E-05	1.47233	2.58E-05	0
40%	Total	15.224515	2.209967	5.50E-05	0.000358	5.49E-05	0.002051	1.670117	5.70E-05	1.710725	3.15E-05	0
50%	Total	25.134264	2.650664	9.40E-05	0.000716	6.96E-05	0.002787	2.047625	0.000115	2.116674	3.77E-05	0
60%	Total	36.382989	3.221718	0.000119	0.000912	9.38E-05	0.004416	2.284749	0.000146	2.39075	4.84E-05	0
70%	Total	64.143953	3.892597	0.000191	0.001507	0.000117291	0.00838	2.795248	0.000241	2.993058	6.68E-05	0
75%	Total	84.744533	4.169869	0.000317	0.002052	0.000126251	0.010753	3.019018	0.000328	3.239403	7.25E-05	0
80%	Total	134.414926	4.60987	0.000377	0.002674	0.000148092	0.021987	3.237884	0.000428	3.729817	8.84E-05	0
85%	Total	173.142736	5.281458	0.000573	0.005205	0.000177063	0.031612	3.527454	0.000833	4.699041	0.000104212	0
90%	Total	202.006796	6.573978	0.001132	0.010531	0.000206529	0.037545	4.349436	0.001685	7.179124	0.000131283	0
95%	Total	451.370159	8.029506	25.126313	236.65387	0.003325593	0.089126	5.719453	37.864619	39.855459	0.000554219	0
97.50%	Total	1074.448414	10.161121	93.571575	1554.778815	0.023450291	0.11341	7.650301	248.76461	252.216628	0.003866483	0
99%	Total	1106.091907	10.526335	190.532886	1644.496244	0.028314339	0.16671	11.081805	263.119399	265.424478	0.004561131	0
99.50%	Total	1224.649416	10.53496	914.590853	5791.737782	0.215570094	0.18496	38.608761	926.678045	927.545556	0.034511826	0
mean	Total	107.3655691	3.30718863	12.95434104	99.59659686	0.00308777	0.01539748	2.74196043	15.93545552	18.69281349	0.000533299	0
sd	Total	229.278764	2.27218729	93.62492806	619.4355337	0.021887665	0.031952714	4.009546426	99.10968536	99.01742054	0.003501366	0
0.50%	Males	0	0.518785	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0
1%	Males	0	0.518785	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0
2.50%	Males	0	0.518785	0	0	7.87E-06	0	0.314057	0	0.321068	4.72E-06	0

SHEDS Technical Manual Section 3.4.2.

The Source Means Output File

Mean Exposure Metrics Across Individuals for Each Source for Chemical

	source.id	exp.dermal	exp.ingest	exp.inhal	dose.inhal	f.dermal	f.ingest	f.inhal	mean.mass
1	P.AC.010.029	0.846165211	0	1.75E-08	1.55E-07	7.55E-06	0	1.39E-12	112046.3292
2	P.AC.010.099	0.541714201	0	1.96E-08	2.00E-07	7.06E-05	0	2.61E-11	7668.754518
3	P.HM.030.099	0	0	0	0	0	0	0	8537179.118
4	P.HM.040.029	4.057914001	0	0	0	2.38E-07	0	0	17023441.25
5	P.PC.220.099	0	0	8.94E-10	8.42E-09	0	0	2.89E-15	2914829.805
6	P.PC.230.099	6860.336636	1.889761369	0.003019375	0.025746509	1.25E-05	3.46E-09	4.71E-11	546758186.3
7	P.PC.240.029	90.91591217	0.035508091	4.09E-05	0.000343764	1.07E-06	4.19E-10	4.06E-12	84735346.94
8	P.PC.240.099	0	0	0.395275995	3.659027672	0	0	0.000139	26373.1226
9	P.PC.250.099	8.228811471	0.00375621	6.648082285	59.72717638	1.72E-06	7.87E-10	1.25E-05	4775601.695
10	P.PC.260.099	1328.24617	0.429937462	0.000529542	0.003893839	2.69E-05	8.72E-09	7.90E-11	49294768.47
11	P.PC.270.099	0.762180036	0	0	0	2.56E-07	0	0	2974737.077
12	P.PC.280.007	371.2598275	0	3.75E-06	4.37E-05	9.21E-05	0	1.08E-11	4029584.897
13	P.PC.280.028	41.49389325	0	7.808998745	74.42123333	6.96E-05	0	0.000125	596102.346
14	P.PC.280.029	0	0	1.10E-07	1.12E-06	0	0	1.40E-12	797188.2943
15	P.PC.280.099	1781.759908	0.681147917	62.1764081	683.8835847	7.87E-05	3.01E-08	3.02E-05	22627342.64
16	P.PC.290.029	0	0	0	0	0	0	0	26496461.25
17	P.PC.290.099	0	0	0	0	0	0	0	210688787.7
18	P.PC.300.099	0	0	0	0	0	0	0	1328.04999
19	P.PC.310.029	0	0	0	0	0	0	0	899507.3629
20	P.PC.310.099	18165.30893	0	0	0	0.125419235	0	0	144836.7068
21	P.PC.320.099	823.1158745	0	4.55E-08	4.11E-07	0.004391182	0	2.19E-12	187447.4356
22	P.PC.830.007	21298.73045	0	4.08E-07	4.26E-06	0.073088471	0	1.46E-11	291410.2634
23	P.PC.830.099	25019.33452	0	5.41E-07	5.18E-06	0.045082713	0	9.33E-12	554965.1471
24	P.PC.840.100	202875.7164	0	5.88E-07	6.66E-06	0.730664291	0	2.40E-11	277659.2739
25	P.PC.840.101	0	0	0	0	0	0	0	68450.75941
26	P.PC.840.029	1453.0524	0	1.20E-07	1.22E-06	0.005842563	0	4.89E-12	248701.2128
27	P.PC.840.099	45941.65627	0	1.16718301	12.73551002	1.018183536	0	0.000282	45121.19344
28	P.PC.850.099	0	0	3.07E-10	5.93E-09	0	0	1.86E-14	318622.0628
29	P.PC.860.099	21819.42934	0	0	0	0.81588435	0	0	26743.28701

SHEDS Technical Manual Section 3.4.2.

Post-Processing For Further Analysis

>combine_output(run.name, out.file, metrics)

- Combines results from **all chemicals** into one file
- run.name -name of run to process
- out.file - filename to create
- metrics – percentiles to include e.g. metrics = c("5%", "50%", "75%", "95%", "99%", "mean", "sd")

CAS	Cohort	exp.derm	exp.inges	exp.inhal_	dose.inha	dose.intal	abs.derma	abs.ingest	abs.inhal.	abs.tot.ug
1912_24_9	Total	0	0.71579	0	0	1.96E-05	0	0.439642	0	0.443794
1912_24_9	Males	0	0.71579	0	0	1.73E-05	0	0.353257	0	0.355344
1912_24_9	Females	0	0.550454	0	0	1.82E-05	0	0.411369	0	0.411369
1912_24_9	Females_Repro	2.09546	0.749056	2.00E-06	1.00E-05	1.53E-05	0.000189	0.370631	2.00E-06	0.370821
1912_24_9	Age_0_5	0	0.550454	0	0	6.82E-05	0	0.591565	0	0.591971
1912_24_9	Age_6_11	0	0.45274	0	0	2.35E-05	0	0.353257	0	0.355344
1912_24_9	Age_12_19	0	1.244437	0	0	1.98E-05	0	0.870716	0	0.875539
1912_24_9	Age_20_65	0	0.834605	0	0	1.73E-05	0	0.411369	0	0.411369
1912_24_9	Age_66+	3.605379	1.917896	1.30E-05	0.000119	2.97E-05	0.000491	1.243752	1.90E-05	1.245435

⋮

SHEDS Technical Manual Section 5.