The Stochastic Human Exposure and Dose Simulation Model: High-Throughput

SHEDS-HT Beta Version 0.1.7

Quick Start Guide

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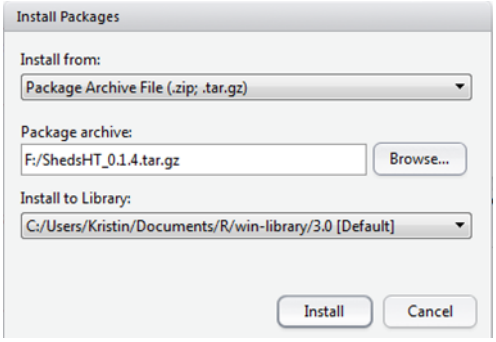
ACKNOWLEDGMENTS AND DISCLAIMER

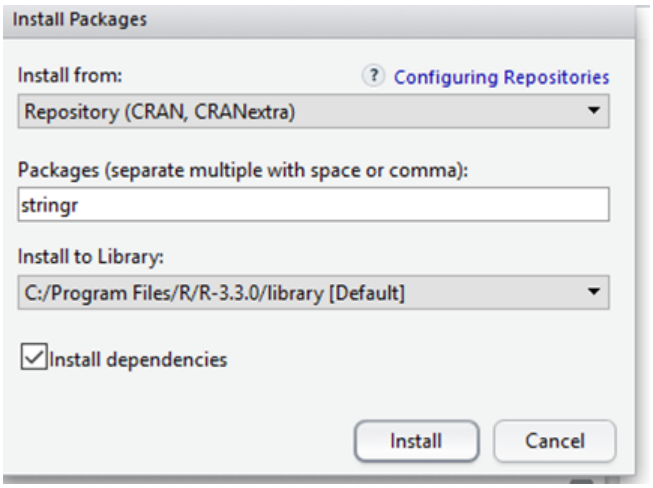
The United States Environmental Protection Agency through its Office of Research and Development funded and collaborated in the research and development of this software, in part under Contract EP-C-14-001 to ICF International. The model is publicly available in Beta version form. All input data used for a given application should be reviewed by the researcher so that the model results are based on appropriate data sources for the given application. This model, default input files, and R package are under continued development and testing. The model equations and approach are published in the peer-reviewed literature (Isaacs et al. Environ. Sci. Technol. 2014, 48, 12750-12759). The data included herein do not represent and should not be construed to represent any Agency determination or policy.

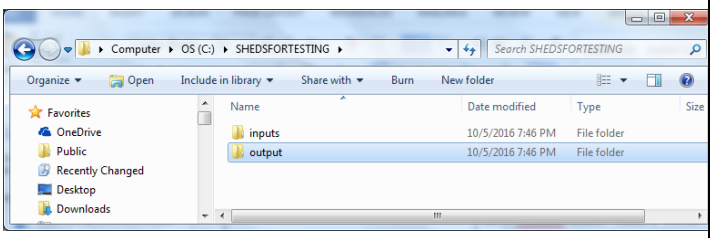
This tutorial will guide you through 1) Installing the SHEDS-HT R Package and corresponding data and 2) running an example run included in the R package (a run of chemicals identified via MSDS sheets as present in various categories of consumer products). This tutorial assumes that you have already:

- Installed R
- Installed RStudio
- Downloaded the most recent version of the SHEDS-HT R package. The most recent SHEDS-Ht release can be obtained https://github.com/HumanExposure/SHEDSHTRPackage. Navigate to the folder "R Package", click on the current file name (e.g., "ShedsHT_0.1.6.tar.gz), and select the "Download" button:

Most of the below steps will only need to be done once. Also included with the SHEDS-HT distribution package is a script titled that, with editing for paths, will perform the steps in this tutorial.

1. Install SHEDS-HT within RStudio	
Start R Studio. Install SHEDS-HT package into your R environment. You will only need to do this once for each computer, or when you are installing an updated version of the R package.	Type the following command into the RStudio command line, giving the path to where ever you stored the SHEDS-HT package file. `>install.packages("F:/ShedsHT_0.1.4.tar.gz", repos = NULL, type = "source")` OR in RStudio, select "Tools"; "Install Packages"; and "Install from: Package Archive File" and browse to the file location. 

Load other R packages required by SHEDS-HT (**data.table**, **stringr**, **plyr**, and **ggplot**). You will only need to do this once for each computer.	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.
	
	 

2. Set up a SHEDS-HT Run	
Create a SHEDS home location for storing your input and output files; create "**inputs**" and "**output**" subfolders. You can create as many SHEDS-HT home folders as you want (with any name), accessing them at different times. Here, for example, we create a folder called "C:/SHEDSFORTESTING"	
Load the ShedsHT Package functions into the current R Studio session. (This must be done every time you start a new R session.)	Type the following command into the RStudio command line: `> library(ShedsHT)`
Run the "**setup**" function on the SHEDS home location folder that you created above, so SHEDS knows where to store materials. (This must be done every time you start a new R session.)	Type the following command into the RStudio command line, using the name of your home directory that you created in Step 1: `> setup("C:/SHEDSFORTESTING")`

If when running "setup()" you receive the message
 	
`Error: cannot open file 'R/Sheds_HT.R': No such file or directory`
 	
Or on some systems:
 	
`Error in file(filename, "r", encoding = encoding) : cannot open the connection`
 	
then you have an old version of SHEDS-HT functions loaded in your R workspace. From the RStudio menu select" Session->Clear Workspace" and try again.
	The version information and EPA Disclaimer will display.
	
	ShedsHT Version 0.1.5 (03/10/2017)
	Disclaimer
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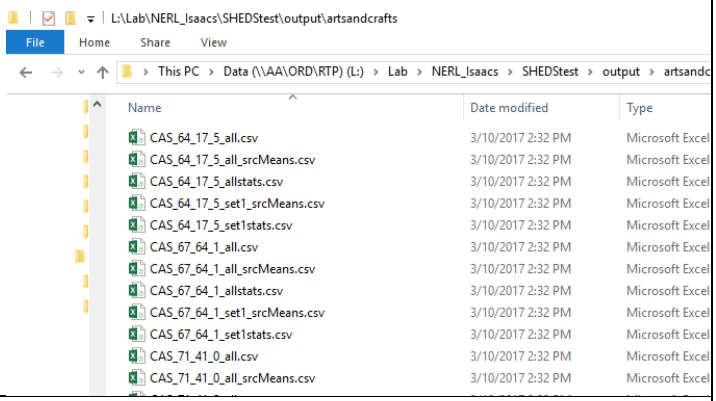
If this is the first time you are using SHEDS, or if you have created a new home location, call **unpack**(). The SHEDS input files included in the R package are written into the "inputs" directory. **If you run unpack() again in the same home location it will overwrite any ShedsHT package input files you have altered.**	Type the following command into the RStudio command line: `> unpack()` This will produce the output: [1] "activity_diaries is exported at c:/SHEDSFORTESTING/inputs/activity_diaries.csv" [1] "chem_props is exported at c:/SHEDSFORTESTING/inputs/chem_props.csv" [1] "diet_diaries is exported at c:/SHEDSFORTESTING/inputs/diet_diaries.csv" [1] "exp_factors is exported at c:/SHEDSFORTESTING/inputs/exp_factors.csv" [1] "fugacity is exported at c:/SHEDSFORTESTING/inputs/fugacity.csv" [1] "media is exported at c:/SHEDSFORTESTING/inputs/media.csv" [1] "physiology is exported at c:/SHEDSFORTESTING/inputs/physiology.csv" [1] "population is exported at c:/SHEDSFORTESTING/inputs/population.csv" [1] "run_artsandcrafts is exported at c:/SHEDSFORTESTING/inputs/run_artsandcrafts.txt" [1] "run_empirical is exported at c:/SHEDSFORTESTING/inputs/run_empirical.txt" [1] "run_foods_1c is exported at c:/SHEDSFORTESTING/inputs/run_foods_1c.txt" [1] "run_others is exported at c:/SHEDSFORTESTING/inputs/run_others.txt" [1] "run_prods_1c is exported at c:/SHEDSFORTESTING/inputs/run_prods_1c.txt" [1] "run_prods_allc is exported at c:/SHEDSFORTESTING/inputs/run_prods_allc.txt" Etc.
3. Perform a SHEDS-HT Run	
Call the SHEDS run function with a SHEDS **Run file** as argument. SHEDS comes with several example run files described in the Technical Manual. They are located in the **input** directory of your SHEDS home location. Here, we run the	`>run("run_artsandcrafts.txt")` This will produce the output: run.name = run_artsandcrafts n.persons = 100 person.output = 1

"**run_artsandcrafts**" example, which runs all the current SHEDS-HT default product composition data for arts and crafts products, which was developed from EPA's CPDat data. Alternatively, one could run all of the default SHEDS-HT data from CPDat (all product types and chemicals) by calling the run "**run_CPDAT**" run file. Note: the **run_CPDAT** run may take 2 or more hours to complete, depending on your computational resources.	source.output = 1 min.age = 0 max.age = 99 genders = M F season = P S F W details = 1 age.match.pct = 20 run.seed = 876144637 set.size = 10000 act.diary.file = Activity_diaries.csv chem.props.file = Chem_props.csv diet.diary.file = Diet_diaries.csv exp.factor.file = Exp_factors.csv fugacity.file = Fugacity.csv media.file = Media.csv physiology.file = Physiology.csv population.file = Population.csv source.vars.file = Source_vars_products.csv source.scen.file = Source_scen_products.csv source.chem.file = source_chem_ac.csv # chemicals = 0 Reading Activity Diaries completed Reading Chemical Properties completed Reading Dietary Diaries completed Reading Exposure Factors completed Reading Media File completed Reading Physiology File completed Reading Population File completed Reading Source.chemicals file completed Reading Source.variables file completed Activity Diary Pooling completed Dietary Diary Pooling completed General Factor Tables completed Media-specific Factor Tables completed Starting source 1 of chem 1 of 24 set= 1 / 1 chem= 1 / 24 100_41_4 ETHYLBENZENE
4. Locate the SHEDS-HT Output Files	
Examine the SHEDS Output files in the Output folder of the SHEDS home folder you designated with **setup**(). The files will be in a subfolder under "Output" with the run name provided in the run file (E.g., either "artsandcrafts" or "CPDat").	
5. Combine SHEDS Output for All Chemicals into a Summary File	

Combine the Percentile Data for all chemicals (i.e. the "AllStats" files created in the output folder) into a single file for other analyses, using the combine_output	`combine_output(run.name="artsandcrafts", out.file="artsandcrafts.csv")`
	
	`Processing chemical 1 of 24`
	`Processing chemical 2 of 24`
	`Processing chemical 3 of 24`
	`Processing chemical 4 of 24`

function, providing a run name. The file is placed in the output folder for the run.	Processing chemical 5 of 24 Processing chemical 6 of 24 Processing chemical 7 of 24 Processing chemical 8 of 24 Processing chemical 9 of 24…