

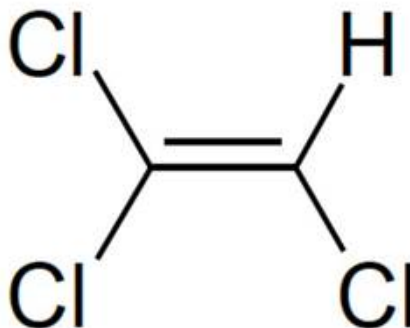


Final Risk Evaluation for Trichloroethylene

Supplemental Information File:

PBPK Model ReadMe

CASRN: 79-01-6



November 2020

The PBPK model files [Risk Evaluation for Trichloroethylene, Supplemental Information File: PBPK Model and ReadMe (zipped).zip] described below are publicly available at the EPA website page for the Final Risk Evaluation for Trichloroethylene, available here: <https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/final-risk-evaluation-trichloroethylene>. These files can be used to recapitulate the model output results used for the PODs utilized in the Risk Evaluation for Trichloroethylene.

README FILE

TCE.1.2.3.3 Directory

- README.docx – This file
- TCE.evaluation.1.2.3.3.pop.model – MCSim model file for MCMC simulations
- TCE.risk5.1.2.3.3.pop.model – MCSim model file for dose metric predictions
- mcsimstd.TCE.evaluation.1.2.3.3.pop.exe – Windows executable for MCMC simulations
- mcsimstd.TCE.risk5.1.2.3.3.pop.exe – Windows executable for dose metric predictions
- ModelResults.R – R script for generating plots of model results
- funcdefs.R – R script with functions used in ModelResults.R script
- OutputVar-labels-plot.csv – CSV file with labels for model outputs

Mouse subdirectory

- Mouse.addldata.Kim.datalabs.txt – data labels for validation data from Kim et al.
- Mouse.check.addldata.Kim-rev.5.pdf – PDF of comparison of model with Kim et al.
- Mouse.check.x.5.pdf – PDF of comparison of distribution of model predictions with calibration data
- Mouse.checkone.5.pdf – PDF of comparison of single random prediction with calibration data
- Mouse.checkone.two.5.pdf – PDF of comparison of distribution of model predictions, and population mean predictions, with calibration data
- Mouse.datalabs.txt – data labels for calibration data
- TCE.1.2.3.3.Mouse.pop.1.5.in – MCMC in file (chain 1)
- TCE.1.2.3.3.Mouse.pop.1.5.out – MCMC out file (chain 1)
- TCE.1.2.3.3.Mouse.pop.2.5.in – MCMC in file (chain 2)
- TCE.1.2.3.3.Mouse.pop.2.5.out – MCMC out file (chain 2)
- TCE.1.2.3.3.Mouse.pop.3.5.in – MCMC in file (chain 3)
- TCE.1.2.3.3.Mouse.pop.3.5.out – MCMC out file (chain 3)
- TCE.1.2.3.3.Mouse.pop.4.5.in – MCMC in file (chain 4)
- TCE.1.2.3.3.Mouse.pop.4.5.out – MCMC out file (chain 4)
- TCE.1.2.3.3.Mouse.pop.check.x.5.in – in file to generate distribution of predictions
- TCE.1.2.3.3.Mouse.pop.check.x.5.out – out file with distribution of predictions
- TCE.1.2.3.3.Mouse.pop.checkone.1.5.in – in file to generate single random prediction
- TCE.1.2.3.3.Mouse.pop.checkone.1.5.out – out file with single random prediction
- TCE.1.2.3.3.Mouse.pop.mean.check.x.5.in – in file to generate population mean predictions
- TCE.1.2.3.3.Mouse.pop.mean.check.x.5.out – out file with population mean predictions
- TCE.1.2.3.3.Mouse.pop.mean.x.5.out – parameter file for population mean predictions
- TCE.1.2.3.3.Mouse.pop.1.4.restart.out – restart file (initial conditions) for MCMC chain 1
- TCE.1.2.3.3.Mouse.pop.2.4.restart.out – restart file (initial conditions) for MCMC chain 2
- TCE.1.2.3.3.Mouse.pop.3.4.restart.out – restart file (initial conditions) for MCMC chain 3
- TCE.1.2.3.3.Mouse.pop.4.4.restart.out – restart file (initial conditions) for MCMC chain 4

Mouse/Parms2 subdirectory:

- TCE.1.2.3.3.Mouse.pop.genparms.setpoints.parmsonly.x.5.out – out file for posterior parameter distributions
- TCE.1.2.3.3.Mouse.pop.genparms.setpoints.x.5.in – in file for parameter distributions
- TCE.1.2.3.3.Mouse.pop.posterior.x.5.dat – parameter file for parameter posteriors
- TCE.1.2.3.3.Mouse.pop.prior.x.5.dat – output file with prior summaries
- TCE.1.2.3.3.Mouse.pop.priors.genparms.setpoints.parmsonly.x.5.out – out file for prior parameter distributions
- TCE.1.2.3.3.Mouse.pop.priors.genparms.setpoints.x.5.in – in file for prior parameter distributions
- TCE.1.2.3.3.Mouse.pop.priors.mc.x.5.in – in file for generating prior scaling parameter
- TCE.1.2.3.3.Mouse.pop.priors.mc.x.5.out – out file of prior scaling parameters
- TCE.1.2.3.3.Mouse.pop.priors.rep500.x.5.out – out file with 500 replicates of scaling parameters

Mouse/PopPred subdirectory

- Mouse.posterior.x.5.pdf – PDF of posterior population distributions
- TCE.1.2.3.3.Mouse.pop.genpop.setpoints.x.5.in – in file for posterior population distributions
- TCE.1.2.3.3.Mouse.pop.genpop.setpoints.x.5.out – out file for posterior population distributions
- TCE.1.2.3.3.Mouse.pop.poppred.addldata.Kim.x.5.out – out file for validation data
- TCE.1.2.3.3.Mouse.pop.poppred.x.5.in – in file for population predictions
- TCE.1.2.3.3.Mouse.pop.poppred.x.5.out – out file for population predictions
- TCE.1.2.3.3.Mouse.pop.x.5.out – parameter file with posterior parameters

Rat.seqpriors.test4 subdirectory

- Rat.seqpriors.test4.addldata.Liu.datalabs.txt – data labels for validation data from Liu et al.
- Rat.seqpriors.test4.addldata.datalabs.txt – data labels for validation data
- Rat.seqpriors.test4.check.addldata.10.pdf – PDF of comparison of model with Liu et al.
- Rat.seqpriors.test4.check.addldata.Liu.10.pdf – PDF of comparison of model with validation data
- Rat.seqpriors.test4.check.x.10.pdf – PDF of comparison of distribution of model predictions with calibration data
- Rat.seqpriors.test4.checkone.10.pdf – PDF of comparison of single random prediction with calibration data
- Rat.seqpriors.test4.checkone.two.10.pdf – PDF of comparison of distribution of model predictions, and population mean predictions, with calibration data
- Rat.seqpriors.test4.datalabs.txt – data labels for calibration data
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.1.10.in – MCMC in file (chain 1)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.1.10.out – MCMC out file (chain 1)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.2.10.in – MCMC in file (chain 2)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.2.10.out – MCMC out file (chain 2)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.3.10.in – MCMC in file (chain 3)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.3.10.out – MCMC out file (chain 3)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.4.10.in – MCMC in file (chain 4)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.4.10.out – MCMC out file (chain 4)
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.check.x.10.in – in file to generate distribution of predictions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.check.x.10.out – out file with distribution of predictions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.checkone.1.10.in – in file to generate single random prediction
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.checkone.1.10.out – out file with single random prediction

- TCE.1.2.3.3.Rat.seqpriors.test4.pop.mean.check.x.10.in – in file to generate population mean predictions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.mean.check.x.10.out – out file with population mean predictions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.mean.x.10.out – parameter file for population mean predictions

Rat.seqpriors.test4/Parms2 subdirectory

- TCE.1.2.3.3.Rat.seqpriors.test4.pop.genparms.setpoints.parmsonly.x.10.out – out file for posterior parameter distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.genparms.setpoints.x.10.in – in file for parameter distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.posterior.x.10.dat – parameter file for parameter posteriors
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.prior.x.10.dat – output file with prior summaries
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.priors.genparms.setpoints.parmsonly.x.10.out – out file for prior parameter distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.priors.genparms.setpoints.x.10.in – in file for prior parameter distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.priors.mc.x.10.in – in file for generating prior scaling parameter
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.priors.mc.x.10.out – out file of prior scaling parameters
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.priors.rep500.x.10.out – out file with 500 replicates of scaling parameters

Rat.seqpriors.test4/PopPred subdirectory

- Rat.seqpriors.test4.posterior.x.10.pdf – PDF of posterior population distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.genpop.setpoints.x.10.in – in file for posterior population distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.genpop.setpoints.x.10.out – out file for posterior population distributions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.poppred.addldata.Liu.x.10.out – out file for validation data
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.poppred.addldata.x.10.in – in file for validation data
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.poppred.addldata.x.10.out – out file for validation data
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.poppred.x.10.in – in file for population predictions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.poppred.x.10.out – out file for population predictions
- TCE.1.2.3.3.Rat.seqpriors.test4.pop.x.10.out – parameter file with posterior parameters

Human.seqpriors.v1 subdirectory

- Human.seqpriors.v1.addldata.datalabs.txt – data labels for validation data
- Human.seqpriors.v1.check.addldata.23.pdf – PDF of comparison of model with validation data
- Human.seqpriors.v1.check.x.23b.pdf – PDF of comparison of distribution of model predictions with calibration data
- Human.seqpriors.v1.checkone.9.pdf – PDF of comparison of single random prediction with calibration data
- Human.seqpriors.v1.checkone.two.23b.pdf – PDF of comparison of distribution of model predictions, and population mean predictions, with calibration data
- Human.seqpriors.v1.datalabs.txt
- TCE.1.2.3.3.Human.seqpriors.v1.pop.1.10.in – MCMC in file (chain 1)

- TCE.1.2.3.3.Human.seqpriors.v1.pop.1.23.out – MCMC out file (chain 1)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.2.10.in – MCMC in file (chain 2)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.2.23.out – MCMC out file (chain 2)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.3.10.in – MCMC in file (chain 3)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.3.23.out – MCMC out file (chain 3)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.4.10.in – MCMC in file (chain 4)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.4.123.out – MCMC out file (chain 4)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.check.x.23.in – data labels for calibration data
- TCE.1.2.3.3.Human.seqpriors.v1.pop.check.x.23.out – in file to generate distribution of predictions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.check.x.23b.out – out file with distribution of predictions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.checkone.1.9.in – in file to generate single random prediction
- TCE.1.2.3.3.Human.seqpriors.v1.pop.checkone.1.9.out – out file with single random prediction
- TCE.1.2.3.3.Human.seqpriors.v1.pop.mean.check.x.23.in – in file to generate population mean predictions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.mean.check.x.23.out – out file with population mean predictions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.mean.x.23.out – parameter file for population mean predictions

Human.seqpriors.v1/Parms2 subdirectory

- TCE.1.2.3.3.Human.seqpriors.v1.pop.genparms.setpoints.parmsonly.x.23.out – out file for posterior parameter distributions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.genparms.setpoints.x.23.in – in file for parameter distributions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.posterior.x.23.dat – parameter file for parameter posteriors
- TCE.1.2.3.3.Human.seqpriors.v1.pop.prior.x.23.dat – output file with prior summaries
- TCE.1.2.3.3.Human.seqpriors.v1.pop.priors.genparms.setpoints.parmsonly.x.23.out out file for prior parameter distributions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.priors.genparms.setpoints.x.23.in – in file for prior parameter distributions
- TCE.1.2.3.3.Human.seqpriors.v1.pop.priors.mc.x.23.in – in file for generating prior scaling parameter
- TCE.1.2.3.3.Human.seqpriors.v1.pop.priors.mc.x.23.out – out file of prior scaling parameters
- TCE.1.2.3.3.Human.seqpriors.v1.pop.priors.rep500.x.23.out – out file with 500 replicates of scaling parameters

ATSDR-comparison subdirectory

- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.1d.inter.setpoints.x.23.in – in file for 1 day intermittent exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.1d.inter.setpoints.x.23.out – out file for 1 day intermittent exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.3wks.inter.setpoints.x.23.in – in file for 3 week intermittent exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.3wks.inter.setpoints.x.23.out – out file for 3 week intermittent exposure

- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.40wks.inter.setpoints.x.23.in – in file for 40 week intermittent exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.40wks.inter.setpoints.x.23.out – out file for 40 week intermittent exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.52wks.setpoints.x.23.in – in file for 52 week continuous exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.52wks.setpoints.x.23.out – out file for 52 week continuous exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.setpoints.x.23.in – in file for 100 week continuous exposure
- TCE.1.2.3.3.Human.seqpriors.v1.pop.noncancer.3.setpoints.x.23.out – in file for 100 week continuous exposure (This file used to calculated summary HEC/HED statistics)
- TCE.1.2.3.3.Human.seqpriors.v1.pop.x.23.out – posterior parameter file
- TCE.risk6.1.2.3.3.pop.model – Model file for dose metrics
- mcsimstd.TCE.risk6.1.2.3.3.pop.static.exe – Windows executable file for model