Readme Describing the Supplementary Information for the Manuscript: Guidance on Evaluating Parametric Model Uncertainty at Decision-Relevant Scales

Jared D. Smith^{1*}, Laurence Lin², Julianne D. Quinn¹, and Lawrence E. Band²

¹University of Virginia, Department of Engineering Systems and Environment ²University of Virginia, Department of Environmental Sciences

*js4yd@virginia.edu

This file describes the contents of all files in the HydroShare data repository entitled "<u>RHESSys</u> <u>Morris Sensitivity Analysis Data Repository for Smith et al.</u>", and provides references to the works cited in the repository files.

S0. S0_CodeAndDataReferences.docx Code and data references, and data processing notes for this paper.

Describes all datasets used for this paper, and provides references to code.

S1. S1_Tables_Fig1&5Data.xlsx: Tables of elementary effects for all model parameters that are plotted in Fig. 1 and 5

This Excel file contains the elementary effects for six decision-relevant and four calibrationrelevant sensitivity metrics, their 90% confidence intervals, and their ranks for all RHESSys parameters displayed in Fig. 1 and 5. This file has three tables (spreadsheets). The BasinOutletEEs_RawValues table contains the raw value of the elementary effects before normalization was completed. The NormalizedAsInFig1&5 table shows the elementary effects after dividing by the maximum P95 value, as shown in Fig. 1 and 5. The Normalized_OnlyNonZeroParams table is the same as the NormalizedAsInFig1&5 table but only shows those parameters with non-zero elementary effects. The last two tables display only two decimal places. All tables share the same column names:

- 1. Parameter Category: The category listed in the Fig. 1 legend.
- 2. Parameter Number: This number indicates the ascending order of parameters along the xaxis in Fig. 1 and 5. Numbers in this field match those placed above the error bars in Fig. 1 and 5.
- 3. Parameter Short Name: The unique name of each parameter as used in the sensitivity analysis. The long names and full descriptions may be found in the Excel file named "Tables_RHESSysParameterDescriptions.xlsx" in this repository. This file is described in S2.
- 4. The following sets of four columns correspond to each of the metrics used to compute elementary effects (Streamflow: Lower 5th Quantiles, Streamflow: 5th to 95th Quantiles, Streamflow: Upper 5th Quantiles, TN: Lower 5th Quantile Estimate, TN: Estimated

Median, TN: Upper 5th Quantile Estimate, LNSE, NSE, Percent Bias, and Log Likelihood). The four columns within these sets display:

- a. P05: The estimated 5th percentile of the elementary effect computed from the bootstrap exercise
- b. Mean: The estimated mean of the elementary effect computed from the bootstrap exercise
- c. P95: The estimated 95th percentile of the elementary effect computed from the bootstrap exercise
- d. Rank: The rank of the parameter's mean value for that metric. Rank 1 is the largest and 103 is the smallest. There are many ties for exactly 0 effect.

S2. S2_Tables_ RHESSysParameterDescriptions.xlsx: Tables describing the RHESSys model parameters.

This Excel file describes all of the RHESSys model parameters used for this study. These include parameters that were varied in the sensitivity analysis and parameters that were fixed (e.g., structural equation choices). This file has three tables (spreadsheets). The Parameters table describes all of the RHESSys parameters that are considered in this study. The CommandLineOptions table describes the command line flags used to run RHESSys. The information presented in these tables was modified from the RHESSys Wiki page (Parameter Definition Files · RHESSys/RHESSys Wiki (github.com), RHESSys command line options · RHESSys/RHESSys Wiki (github.com)). The final table is OnlySAparams and includes a simplified table with only parameters and their lower and upper bounds that were used in the sensitivity analysis.

The *CommandLineOptions table* has the following columns:

- 1. Type: Indicates how the flag affects the model. Options are:
 - a. Required: RHESSys will not successfully run without these
 - b. Output: Tells RHESSys how output should be reported
 - c. Hydrology: Describes how water should be routed among patches
 - d. Sensitivity Multipliers: Multipliers to the def file parameter values.
 - e. Soil: Describes additional water routing options and biogeochemical processes
 - f. Climate: Describes climate data specifications, and which processes are modeled
 - g. Fire: Allows modeling of fire spreading
 - h. Land Use: Options for land use processes
 - i. Vegetation: Specifies if growth mode should be used, and various other processes.
 - j. Debug: Options to print verbose output.
- 2. Flag: The command line flag
- 3. Description: Describes what the flag does to the RHESSys model
- 4. Possible Values: Describes the range of possible values to use
- 5. Default in RHESSys If Not Specified: What RHESSys will use for the flag if it's not specified.
- 6. Used in paper?: y indicates that the flag was used in this paper. The value used is reported in the Parameters table under the Command Line heading.

The *Parameters table* is split into several sections, one for each category of RHESSys parameters. The categories are: Command Line, Hillslope, Zone, Soil, Land Use, and Vegetation. Each category has the following columns:

- 1. Parameter: The parameter name
- 2. Description: A description of what the parameter affects in RHESSys
- 3. Unit: The expected unit of the parameter value
- 4. Lower Bound: The assigned lower bound of the uniform distribution used in the sensitivity analysis. Only applies to parameters that were varied.
- 5. Upper Bound: The assigned upper bound of the uniform distribution used in the sensitivity analysis. Only applies to parameters that were varied.
- 6. Fixed Value: The value assigned to a parameter that was held constant in the sensitivity analysis.
- 7. Notes: Contains references to literature and descriptions that support the choice of parameter bounds and fixed values.
- 8. Default Value: The value that RHESSys would assign to the parameter if no value is specified by the user. These are reported in this spreadsheet because some parameter bounds are based on a percentage of the default value. The default value for command line parameters is reported on that table.

Parameters that were aggregated because of known physical relations and mathematical constraints have one additional column filled in:

9. Aggregated Parameter Name: The name of the aggregated parameter that corresponds to the Parameter in the same row.

Categories that have multiple types (soils, vegetation, land use) require a separate def file for each type. Many parameters share the same bounds and fixed values across types, and those are reported in the same columns as listed above. For those parameters whose values differ between types, we list "Type Specific" in the columns above, and separately report the lower and upper bounds for the parameters in the following columns:

10. Lower Bound column name beneath a merged cell containing the specific type name

11. Upper Bound column name beneath a merged cell containing the specific type name

The **OnlySAparams table** has the following columns:

- 1. NumberedParams: provides a unique parameter name to all parameters for use in the sensitivity analysis. Unique names append category indicators to the start of the parameter name. These include: h, l, z, s8, s108, s9, s109, v3, v4, or v102 for hillslope, land use, zone, soil 8, soil 108, soil 9, soil 109, vegetation 3, vegetation 4, vegetation 102, respectively.
- 2. DefParameter: Name of the parameter as required by RHESSys.
- 3. Lower: The lower bound from the previous table.
- 4. Upper: The upper bound from the previous table.

The selected parameters apply to the following model structures that are selected as fixed parameters in RHESSys:

Soil:

- No rain-on-snow pooling models of heat transfer. This is the default option, and limited data are available to inform these parameters
- AGE albedo model instead of the BATS model.
- Clapp-Hornberger hydraulic conductivity equations instead of Van Genuchten equations.

Zone:

• atmospheric transmissivity is not considered to vary seasonally (the annual parameter is used instead of seasonal)

Hillslope:

• A fast groundwater storage is not used because this watershed has fairly thick bedrock and is vegetated such that slow storage is more likely.

Land Use:

- No septic nitrate loading and no fertilization because nitrogen is modeled with WRTDS.
- No grazing because there are no farms in the Baisman Run watershed.
- Irrigation is not modeled.

Vegetation:

- No canopy heat transfer model.
- Temperature acclimation of respiration Q10 is not used (Tjoelker et al., 2001).
- Used annual instead of daily allocation of maintenance respiration.
- Dickenson carbon allocation strategy is used instead of Waring.

Zone Parameter Citations

(Bristow & Campbell, 1984), (Hungerford et al., 1989), (Longman et al., 2012), (NREL, 2012), (Muleta & Nicklow, 2005), (Jennings et al., 2018), (Kaushal et al., 2011), (Campbell et al., 2019), (Lima et al., 2019; López et al., 2019; Zhang et al., 2019)

Hillslope Parameter Citations

(Winter et al., 1998)

Soil Parameter Citations

(Dingman, 1994, p. 222; García-Gutiérrez et al., 2018), (Dai et al., 2019), (Williams & Flanagan, 1996), (Froelich, 1975; Reybold & Matthews, 1976), (Clapp & Hornberger, 1978), (Molotch & Bales, 2006)

Vegetation Parameter Citations

(Leonard et al., 2017; Lin, 2019; Miles, 2015a, 2015b), (Hawkins et al., 2019), (White et al., 2000), (Berg & McClaugherty, 2003; Cross et al., 2005; Lin et al., 2015), (Jolly et al., 2005), (Ryan, 1991), (Landsberg & Waring, 1997), (Tjoelker et al., 2001), (Arora & Boer, 2003)

S3. S3_satDefRepsBasin_Med.png Saturation deficit over time in the RHESSys simulation.

This figure is provided to support the choice of using 5 years to spin-up the RHESSys model's water storage levels. RHESSys begins a simulation with the water table at the surface (0 saturation deficit). In this plot, the saturation deficit is plotted for all model runs in light, transparent gray, and the red line in this figure is the median. Darker areas have a higher density of model runs. Most runs have reached a more stable saturation deficit value after 5 years.

S4. S4_HillEERanksAllMetrics folder

Figure 3C elementary effect ranks for each other streamflow sensitivity metric.

Files: HillRankTop1295_05s_Aggh_paper_g.png, HillRankTop1295_ots_Aggh_paper_g.png,

These figures correspond to streamflow 5th percentile (05s) and 5th-95th percentile (ots). Figures are also provided in the folder for streamflow 05s and ots using the annual 5th percentile (filenames for 05s and ots without _g at the end). The paper figures for 95th percentile streamflow are also provided for reference.

S5. S5_MultipliersForAllMetrics folder Figure 4 multiplier evaluation for each other sensitivity metric.

Files: BasinAllMultEEs_05s_g.png, BasinAllMultEEs_ots_g.png, BasinAllMultEEs_TN05.png, BasinAllMultEEs_TN95.png, BasinAllMultEEs_TNMed.png

These figures correspond to streamflow 5th percentile (05s), 5th-95th percentile (ots), TN 5th quantile estimates (TN05), TN 95th quantile estimates (TN95), and log-space mean TN (real space median) (TNMed). Figures are also provided in the folder for streamflow 05s and ots using the annual 5th percentile (filenames for 05s and ots without _g at the end).

S6. S6_WRTDS folder WRTDS Interpolation Tables and Figures

A subfolder provides the interpolation tables used to estimate TN from the simulated streamflow and day of the year. Figures of those tables are also provided in that folder.

Figures in the WRTDS folder provide the estimated mean TN concentration and flux over time, and 1 error standard deviation.

S7. S7_MetricScatterplotMatrix folder Scatterplot matrix of all sensitivity metrics evaluated at the basin outlet.

The lower right triangle provides scatterplots that are density shaded (darker = more points), the diagonal provides histograms of the labeled metric, and the upper right triangle provides correlation coefficients (Pearson on one figure and Spearman rank correlation on another). There is one point for each model run completed in the sensitivity analysis. Labels are logL: log likelihood, LNSEd: Nash-Sutcliffe efficiency for the natural log of daily flows, NSEd: Nash-Sutcliffe efficiency for daily flows, pBias: percent bias for streamflows, SAE05g: sum of absolute error for the 5th percentile streamflow metric computed over the historical record, SAEotg: sum of absolute error for the 5th to 95th percentiles streamflow metric, SAETN05: sum of absolute error for the 5th error quantile of TN, SAETNMed: sum of absolute error for the 7th error quantile of TN.

PaperFigures

Contains the figures found within the paper. The AnnualLower5thPercentile directory contains the figures that resulted from using the annual 5th percentile instead of the 5th percentile over the historical record.

Also includes the svg files used to make figures in Inkscape, and the GoogleEarth files used to make some figures.

SAData

Contains the RData file with all of the RHESSys and WRTDS model output, and Morris elementary effects for all sensitivity analysis runs. The readme file in this directory explains how to obtain the paper figures, as found in the PaperFigures directory.

RHESSysData

Contains the data and code used to obtain the files in SAData. The code and the workflow to run the code are described in the GitHub repository for this paper. See S0 for the citation to the GitHub code repository: RHESSys_ParamSA-Cal-GIOpt.

References

- Arora, V. K., & Boer, G. J. (2003). A Representation of Variable Root Distribution in Dynamic Vegetation Models. *Earth Interactions*, 7(6), 1–19. https://doi.org/10.1175/1087-3562(2003)007<0001:AROVRD>2.0.CO;2
- Berg, B., & McClaugherty, C. (2003). *Plant Litter: Decomposition, Humus Formation, Carbon Sequestration*. Springer.
- Bristow, K. L., & Campbell, G. S. (1984). On the relationship between incoming solar radiation and daily maximum and minimum temperature. *Agricultural and Forest Meteorology*, *31*(2), 159–166. https://doi.org/10.1016/0168-1923(84)90017-0
- Campbell, P. C., Bash, J. O., Nolte, C. G., Spero, T. L., Cooter, E. J., Hinson, K., & Linker, L. C. (2019). Projections of Atmospheric Nitrogen Deposition to the Chesapeake Bay Watershed. *Journal of Geophysical Research: Biogeosciences*, 124(11), 3307–3326. https://doi.org/10.1029/2019JG005203
- Clapp, R. B., & Hornberger, G. M. (1978). Empirical equations for some soil hydraulic properties. *Water Resources Research*, 14(4), 601–604. https://doi.org/10.1029/WR014i004p00601
- Cross, W. F., Benstead, J. P., Frost, P. C., & Thomas, S. A. (2005). Ecological stoichiometry in freshwater benthic systems: recent progress and perspectives. *Freshwater Biology*, *50*(11), 1895–1912. https://doi.org/10.1111/j.1365-2427.2005.01458.x
- Dai, Y., Xin, Q., Wei, N., Zhang, Y., Shangguan, W., Yuan, H., Zhang, S., Liu, S., & Lu, X. (2019). A Global High-Resolution Data Set of Soil Hydraulic and Thermal Properties for Land Surface Modeling. *Journal of Advances in Modeling Earth Systems*, 11(9), 2996– 3023. https://doi.org/10.1029/2019MS001784
- Dingman, S. L. (1994). *Physical Hydrology*. Macmillan Publishing Company. https://books.google.com/books?id=MRMSAQAAIAAJ
- Froelich, A. J. (1975). *Bedrock Map of Montgomery County, Maryland*. https://doi.org/Miscellaneous Geologic Investigations Map I-920-D
- García-Gutiérrez, C., Pachepsky, Y., & Martín, M. Á. (2018). Technical note: Saturated hydraulic conductivity and textural heterogeneity of soils. *Hydrology and Earth System Sciences*, *22*(7), 3923–3932. https://doi.org/10.5194/hess-22-3923-2018
- Hawkins, L. R., Rupp, D. E., McNeall, D. J., Li, S., Betts, R. A., Mote, P. W., Sparrow, S. N., & Wallom, D. C. H. (2019). Parametric Sensitivity of Vegetation Dynamics in the TRIFFID Model and the Associated Uncertainty in Projected Climate Change Impacts on Western U.S. Forests. *Journal of Advances in Modeling Earth Systems*, *11*(8), 2787–2813. https://doi.org/10.1029/2018MS001577

- Hungerford, R. D., Nemani, R. R., Running, S. W., & Coughlan, J. C. (1989). MTCLIM: a mountain microclimate simulation model. In *Research Paper - US Department of Agriculture, Forest Service* (Issue INT-414). https://doi.org/10.2737/INT-RP-414
- Jennings, K. S., Winchell, T. S., Livneh, B., & Molotch, N. P. (2018). Spatial variation of the rain–snow temperature threshold across the Northern Hemisphere. *Nature Communications*, 9(1), 1148. https://doi.org/10.1038/s41467-018-03629-7
- Jolly, W. M., Nemani, R., & Running, S. W. (2005). A generalized, bioclimatic index to predict foliar phenology in response to climate. *Global Change Biology*, *11*(4), 619–632. https://doi.org/10.1111/j.1365-2486.2005.00930.x
- Kaushal, S. S., Groffman, P. M., Band, L. E., Elliott, E. M., Shields, C. A., & Kendall, C. (2011). Tracking Nonpoint Source Nitrogen Pollution in Human-Impacted Watersheds. *Environmental Science & Technology*, 45(19), 8225–8232. https://doi.org/10.1021/es200779e
- Landsberg, J. J., & Waring, R. H. (1997). A generalised model of forest productivity using simplified concepts of radiation-use efficiency, carbon balance and partitioning. *Forest Ecology and Management*, 95(3), 209–228. https://doi.org/10.1016/S0378-1127(97)00026-1
- Leonard, L., Lin, L., & Band, L. E. (2017). *DeadRun Definition Files*. Hydroshare. https://www.hydroshare.org/resource/b60c5fa950ee401fac8a6ef0f1d0c441/
- Lima, A. O., Lyra, G. B., de Souza, J. L., Lyra, G. B., de Oliveira-Júnior, J. F., & Santos, A. A. R. (2019). Assessment of monthly global solar irradiation estimates using air temperature in different climates of the state of Rio de Janeiro, Southeastern Brazil. *SN Applied Sciences*, *1*(9), 1002. https://doi.org/10.1007/s42452-019-1041-z
- Lin, L. (2019). GIS2RHESSys. https://github.com/laurencelin/GIS2RHESSys
- Lin, L., Webster, J. R., Hwang, T., & Band, L. E. (2015). Effects of lateral nitrate flux and instream processes on dissolved inorganic nitrogen export in a forested catchment: A model sensitivity analysis. *Water Resources Research*, 51(4), 2680–2695. https://doi.org/10.1002/2014WR015962
- Longman, R. J., Giambelluca, T. W., & Frazier, A. G. (2012). Modeling clear-sky solar radiation across a range of elevations in Hawai'i: Comparing the use of input parameters at different temporal resolutions. *Journal of Geophysical Research: Atmospheres*, *117*(D02201), 1–13. https://doi.org/10.1029/2011JD016388
- López, M. L., Olcese, L. E., Palancar, G. G., & Toselli, B. M. (2019). Accurate total solar irradiance estimates under irradiance measurements scarcity scenarios. *Environmental Monitoring and Assessment*, 191(9), 568. https://doi.org/10.1007/s10661-019-7742-3
- Miles, B. (2015a). Dead Run 5, Catonsville, MD RHESSys model. In *Hydroshare*. https://www.hydroshare.org/resource/895cc2fc795f4a63ab35c291d39977dc
- Miles, B. (2015b). *RHESSys model of Dead Run 5 watershed, Baltimore County, Maryland, USA (with rain gardens)*. Hydroshare. https://www.hydroshare.org/resource/6dbb0dfb8f3a498881e4de428cb1587c/

- Molotch, N. P., & Bales, R. C. (2006). Comparison of ground-based and airborne snow surface albedo parameterizations in an alpine watershed: Impact on snowpack mass balance. *Water Resources Research*, 42(5), 1–12. https://doi.org/10.1029/2005WR004522
- Muleta, M. K., & Nicklow, J. W. (2005). Sensitivity and uncertainty analysis coupled with automatic calibration for a distributed watershed model. *Journal of Hydrology*, *306*(1–4), 127–145. https://doi.org/10.1016/j.jhydrol.2004.09.005
- NREL. (2012). United States Annual Average Wind Speed at 30 m (p. 1). https://windexchange.energy.gov/maps-data/325
- Reybold, W. U. 'III', & Matthews, E. D. (1976). *Soil Survey of Baltimore County, Maryland*. https://www.nrcs.usda.gov/Internet/FSE_MANUSCRIPTS/maryland/baltimoreMD1976/bal timoreMD1976.pdf
- Ryan, M. G. (1991). Effects of Climate Change on Plant Respiration. *Ecological Applications*, *1*(2), 157–167. http://www.jstor.org/stable/1941808
- Tjoelker, M. G., Oleksyn, J., & Reich, P. B. (2001). Modelling respiration of vegetation: evidence for a general temperature-dependent Q 10. *Global Change Biology*, 7(2), 223–230. https://doi.org/10.1046/j.1365-2486.2001.00397.x
- White, M. A., Thornton, P. E., Running, S. W., & Nemani, R. R. (2000). Parameterization and Sensitivity Analysis of the BIOME–BGC Terrestrial Ecosystem Model: Net Primary Production Controls. *Earth Interactions*, 4(3), 1–85. https://doi.org/10.1175/1087-3562(2000)004<0003:PASAOT>2.0.CO;2
- Williams, T. G., & Flanagan, L. B. (1996). Effect of Changes in Water Content on Photosynthesis, Transpiration and Discrimination against 13CO2 C18O16O in Pleurozium and Sphagnum. *Oecologia*, 108(1), 38–46. https://doi.org/https://www.jstor.org/stable/4221384
- Winter, T. C., Harvey, J. W., Franke, O. L., & Alley, W. M. (1998). Groundwater and surface water: A single resource. In USGS Circular 1139. https://pubs.usgs.gov/circ/circ1139/
- Zhang, Y., Cui, N., Feng, Y., Gong, D., & Hu, X. (2019). Comparison of BP, PSO-BP and statistical models for predicting daily global solar radiation in arid Northwest China. *Computers and Electronics in Agriculture*, 164(July), 104905. https://doi.org/10.1016/j.compag.2019.104905