Quantitative Microbial Risk Assessment Tutorial

Primer

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Summary

This document provides a Quantitative Microbial Risk Assessment (QMRA) primer that organizes QMRA tutorials. The tutorials describe functionality of a QMRA infrastructure, guide the user through software use and assessment options, provide step-by-step instructions for implementing a mixed-use, watershed-based QMRA, and suggest the order for reading and reviewing the tutorials.

Primer

PURPOSE

An integrated environmental modeling infrastructure has been developed to automate data acquisition to meet data input requirements of a confederation of models and to execute these models within a system workflow. The purpose of this document is to describe what support documentation is available to help train users in the use and application of the software.

OBJECTIVE

The objective is to describe the individual instructional tutorials that provide step-by-step documentation for implementing a mixed-use, watershed-based Quantitative Microbial Risk Assessment (QMRA), as illustrated in Figure 1. This results in a series of software tools that automate many of the manual steps associated with a standard watershed assessment that collectively expedite the process, minimize resource requirements, increase ease of use, and bring more science-based processes into the analysis. Technically, the software and documentation

- Provide a watershed-based capability
- Allow users to inspect time series of water flows and microbial densities at multiple watershed locations
- Incorporate process-based science
- Use existing U.S. Environmental Protection Agency (EPA) and Office of Water (OW) modeling tools
- Allow for the inclusion of other software components

OUTPUT

A QMRA Primer that organizes QMRA tutorials which describe functionality of a QMRA infrastructure, guide the user through software use and assessment options, provide step-by-step instructions for implementing a mixed-use, watershed-based QMRA, and suggest the order for reading and reviewing the tutorials.

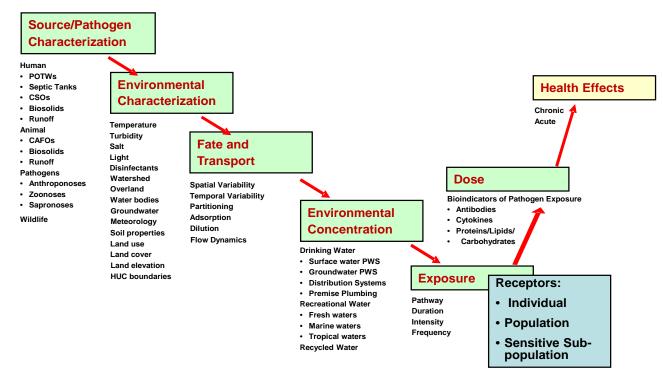


Figure 1. Mapping a microbial risk assessment based on human-health impacts to EPA National Exposure Research Laboratory Exposure Science (After Araujo et al., 2009; Villegas, 2013)

TABLE OF CONTENTS

QUANTITATIVE MICROBIAL RISK ASSESSMENT

COMPONENTS OF A QMRA MODELING SYSTEM

QMRA MODELING WORKFLOW

QMRA DOCUMENTATION

DISCLAIMER

ACKNOWLEDGMENTS

REFERENCES

QUANTITATIVE MICROBIAL RISK ASSESSMENT

A Quantitative Microbial Risk Assessment (QMRA) is a modeling approach that integrates disparate data, including those linked to microbial fate/transport and exposure, and human health-effect relationships to characterize potential health impacts/risks from exposure to pathogenic microorganisms (Soller et al., 2010; Whelan et al., 2014a, 2014b; Haas et al., 1999; Hunter et al., 2003). As Whelan et al. (2014b) note, a QMRA's conceptual design fits well within an integrated, multi-disciplinary modeling perspective (illustrated in Figure 2). The approach describes the problem statement, data access retrieval and processing [e.g., D4EM (EPA, 2013a; Whelan et al., 2009; Wolfe et al., 2007)]; software frameworks for integrating models and databases [e.g., FRAMES (Johnston et al., 2011)]; infrastructures (or frameworks) for performing sensitivity, variability, and uncertainty analyses (Babendreier and Castleton, 2005); and risk quantification. By coupling modeling results with epidemiology studies, policy-related issues (e.g., EPA, 2010; EPA and USDA, 2012) can be explored (Figure 2).

Experience shows that a substantial amount of time is required to set up the Conceptual Site Model (CSM), collect data that meet model input requirements, and populate model input files prior to any model execution, leaving less time and resources for actual analysis. A CSM or system conceptualization captures the essence of the real-world problem including the processes, cycles, and flows that characterize the relevant environmental components of the system (Fischenich, 2008; Laniak et al., 2013). The CSM provides substance to the components outlined in Figure 2. Because QMRAs can be considered a microbial version of the existing chemical risk paradigm (Whelan et al., 2014b; EPA 2012a, 2012b), manual procedures to collect data from standard databases (e.g., NHDPlus, NLCD, NLDAS, etc.) and populate model input files tend to be repeated, lending themselves to automation. This is consistent with Laniak et al. (2013) and Peckham et al. (2013) who noted a near-term need is to automate data-gathering by meeting input model data requirements and model-coupling processes as much as possible (Whelan et al., 2014c). A watershed-scale microbial source-to-receptor workflow is constructed that follows the release of microbes from animal-impacted catchments through its waterbody network to receptors of concern. Our objective is to automate the manual steps associated with this standard QMRA-based watershed assessment, and thereby expedite the process, minimize resource requirements, increase ease of use, and bring more science-based processes to the analysis.

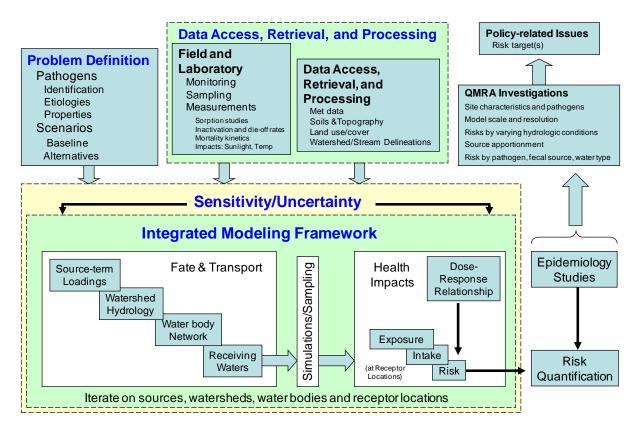


Figure 2. One rendition of QMRA from an integrated, multi-disciplinary multimedia modeling framework perspective that links problem definition; data access, retrieval, and processing; integrated modeling framework with source-to-receptor environmental models, housed within a sensitivity/uncertainty software structure; and risk quantification linked to epidemiology studies and policy-related uses (After Whelan et al., 2014b).

COMPONENTS OF A QMRA MODELING SYSTEM

Nine models and data files form a loosely configured modeling infrastructure that supports watershed-scale microbial source-to-receptor modeling that focuses on animal-impacted catchments. Components of a QMRA modeling system are described as follows:

- Microbial Input: Includes properties of microorganisms and information related to microbial sources
 - Properties Data: Capture microbial-related properties of microorganisms, as well as data related to the release of microorganisms associated with fecal material. Microbial properties data are housed within eight default local data Excel files which allow users to modify values of parameters that impact the release, migration, fate, and transport of microbes within a watershed, and control its delineation into subwatersheds.
 - Microbial Source Files: Contain microbial source locations, animal numbers and types, correlated with land-use type within subwatersheds. Although there is no user-friendly interface to manage them, these five files allow users to identify specific locations of domestic animals, sampling/monitoring, septic systems, and point sources [e.g., Publicly Owned Treatment Works (POTWs) and Wastewater Treatment Plants (WWTPs)].

Currently, these data need to be manually researched and compiled within pre-formatted Excel spreadsheets. Although a user-friendly interface to manage them does not yet exist, these files allow users to modify input parameters that directly impact microbial loadings to a watershed. The files are included in the software download, during installation, and stored within the working folder on the user's personal computer, when it is created during execution of the QMRA software (Whelan et al., 2017a).

- Data for Environmental Modeling (D4EM): D4EM manages, accesses, retrieves, analyzes, and caches web-based environmental data. D4EM (Wolfe et al., 2007; Aqua Terra, 2011; EPA, 2013a) (1) is an Open Source automated data access and processing library that accesses a variety of data types including water quality, land use, hydrology, soils, meteorological (MET), stream flow, groundwater levels, and crop data; (2) uses DotSpatial geo-processing libraries (CodePlex, 2014) to perform cartographic re-projections, intersection, clipping, overlaying, joining and merging of geographic features, and areas-of-interest delineation; (3) performs statistical processing (extraction, interpolation and averaging) of time series data; (4) incorporates automatic data access functionality; and (5) consists of a collection of .Net dynamic link libraries that can be linked to a modeling utility such as a batch processor or script to access data for multiple sites, or used with a custom-built user interface such as the SDMProjectBuilder.
- Microbial Source Module (MSM): The MSM organizes, analyzes, and supplies the necessary data to determine microbial loading rates within a watershed to support HSPF input data requirements (Whelan et al., 2017b), and is based on the HSPF Bacterial Indicator Tool (EPA, 2013b, 2013c). The MSM works with the SDMProjectBuilder to read a pre-populated file with microbial source locations, animal numbers and types [agricultural animals (cattle, swine, poultry, etc.), wildlife (ducks, deer, etc.), manure application schedules, grazing patterns, and point source releases (e.g., septic systems and treatment facilities), where applicable] by latitude-longitude and correlate them with land-use type (i.e., built-up/impervious, pastureland, cropland, or forest) and subwatersheds delineated by the SDMProjectBuilder. The MSM develops microbial loadings, adjusted for die-off, to the overland (e.g., counts/ha/d) by land use and month and instream (counts/hr) locations within a watershed, and automatically pre-populates the HSPF User Control Input (UCI) file with microbial loading rates. Time scales for instream, point-source loadings can vary.
- **Site Data Manager Project Builder (SDMProjectBuilder):** The SDMProjectBuilder leverages D4EM to manage access, retrieval, analysis, and caching of web-based environmental data (e.g., NHDPlus,

NLCD, NCDC, STORET, NLDAS, STATSGO/SSURGO, etc.); provides geographical information system (GIS) capabilities using DotSpatial technology; converts DotSpatial-based project files to MapWindow-based project files (MapWindow 2011, 2013; Watry and Ames, 2008); and automatically pre-populates input files of fate and transport models. It automates the watershed delineation process, allowing for 8-digit and 12-digit Hydrologic Unit Codes (HUC-8 and HUC-12, respectively) or pour point analyses; assigns map-layer features automatically [e.g., slope, soil, land use, microbial sources, National Climatic Data Center (NCDC) and North American Land Data Assimilation System (NLDAS) (Kim et al., 2014) MET stations (Whelan et al., 2017c)]; and accounts automatically for snow accumulation/melt, microbial fate and transport, and user-defined simulation time increments (e.g., hourly, daily, monthly, or annually) (Whelan et al., 2017d, 2017e, 2017f, 2017g). The ability to define time increments is valuable, especially when hourly storm events drive an assessment.

- Hydrologic Simulation Program FORTRAN (HSPF): HSPF (Bicknell et al., 1997) is software program for simulating watershed hydrology and water quality for conventional (such as sediment or nutrients) and nonconventional (such as toxic organic) pollutants and microbes, with microbes as the focus; implements a basin-scale analysis that includes hydrology and water quality to allow integrated simulation of land and soil contaminant runoff processes with instream hydraulic and microbial interactions on user-defined time scales (hour, day, month, or year); and provides a time history of runoff flow rates and microbial concentrations at any point in a watershed (EPA, 2013d). HSPF simulates flow, microbial, and chemical fate/transport within a watershed and executes as a stand-alone or from within BASINS.
- Parameter ESTimation and Uncertainty Analysis (PEST): The model-independent PEST is a nonlinear parameter estimation package that can estimate parameter values for almost any existing computer model, whether a user has access to the model's source code (SSPA, 2010; C⁴Site Factory, 2011; Doherty, 2005) or not. PEST is designed to interface with an existing model, modify designated input, run the model as often as needed, and adjust its parameters until differences between simulated and monitored output results are minimized in a weighted least squares sense. PEST communicates with a model through the model's own input and output files. PEST implements a variant of the Gauss-Marquardt-Levenberg method of nonlinear parameter estimation (Doherty, 2005).
- Better Assessment Science Integrating point & Non-point Sources system (BASINS): BASINS (EPA, 2001; Lahlou et al., 1998) is a multipurpose environmental analysis infrastructure that performs watershed- and water quality-based analyses by integrating environmental data, analysis tools, and watershed and water quality models. A MapWindow-based GIS organizes spatial information that displays maps, tables, or graphics; analyzes landscape information; and integrates and displays relationships among data at a user-chosen scale (EPA, 2013e). With this QMRA context, BASINS provides graphical and tabular viewers of flow and concentration output.
- San Antonio River Authority (SARA) Timeseries Utility: The SARA Timeseries Utility supports analysis and management of time-varying environmental data including listing, graphing, computing statistics, computing MET data, and saving in a WDM or text file (Aqua Terra, 2011). Supported file formats include: WDM, HSPF Binary (.hbn), USGS RDB, and text files, using the same import scripts as WDMUtil and BASINS. Users of WDMUtil will find most of its functionality is included in this new utility tool which allows users to publish HSPF data as a txt file for consumption by other components (Whelan et al., 2017h).
- Microbial Risk Assessment—Interface Tool (MRA-IT): MRA-IT is a MathCad-based, integrated software tool based on the pathogen of interest, exposure, intake, and dose (Whelan et al., 2014b; Soller et al., 2008, 2004; Soller and Eisenberg, 2008). MRA-IT consumes a series of pathogenic densities from a text (.txt) file like that produced by the SARA Timeseries Utility (Whelan et al.,

2017h) and characterizes human-health risk from ingestion of reclaimed water through recreational activities, consumption of crops irrigated with reclaimed water, or incidental/inadvertent ingestion of reclaimed water associated with golf course/landscape irrigation. Key components include, but are not limited to, pathogen specification, exposure scenario identification, and dose-response relationships.

QMRA MODELING WORKFLOW

A QMRA infrastructure that automates the manual process of characterizing transport of pathogens and microorganisms, from the source of release to a point of exposure, has been developed by loosely configuring a set of modules and process-based models. A design schematic of the workflow, tracking data from sources to risk assessment and visualization of simulation results, is presented in Figure 3.

- 1. The user initiates the SDMProjectBuilder process by navigating the United States by state, county, and HUC-8, and selecting the HUC-8 of interest (Whelan et al., 2017d). A HUC-8 is typically a watershed with an area of 700 mi².
- 2. The SDMProjectBuilder registers 12 Excel-based microbial input data files, sometimes referred to as Local Data files, containing microbial-related properties and locations for sources of contamination (Whelan et al., 2017a).
- 3. The SDMProjectBuilder manages data acquisition from standard national databases using D4EM which is based on the BASINS watershed modeling system data-download tool. The result is a delineated watershed containing a suite of GIS map layers that include NHDPlus flowlines, waterbodies, and catchments (subwatersheds); waterbody network; elevation (e.g., slope); soil types; land use types; MET stations; and multiple legal boundaries (state, county, roads, eco/NAWQA regions, etc.). Many map layers are similar to those found in BASINS. With user-defined simulation output time intervals (hourly, daily, etc.), simulation start and end times, and selected data sources, the SDMProjectBuilder delineates the watershed of interest into smaller subwatersheds when a HUC-12 (Whelan et al., 2017e) or pour point (Whelan et al., 2017f) is chosen. A HUC-12 is typically a watershed between 16 and 63 mi². Users also can control subwatershed and land-use-type sizes, and flow lengths.
- 4. Working with SDMProjectBuilder, the MSM (Whelan et al., 2017b) consumes potential microbial source locations/types and overlays them on subwatersheds, creating microbial loadings for each subwatershed and stream reach.
- 5. Coupled with other acquired data, the SDMProjectBuilder automatically creates input files for various models (HSPF in this case, as shown in Figure 3), a collection of geospatial data files, and a MapWindow project (.mwprj) file currently used by BASINS (Figure 3) (Whelan et al., 2017e, 2017f, 2017g).
- 6. Using the HSPF Windows interface, non-spatially related data may be modified. For example, if a point source exists within the watershed, its loadings can be registered within HSPF prior to execution (Whelan et al., 2017g).
- 7. HSPF is executed, creating flows and microbial concentrations spatially and temporally distributed throughout the watershed (Whelan et al., 2017e, 2017f, 2017g).
- 8. PEST is executed, providing a calibration of HSPF flow and microbial fate and transport simulations. Initial estimates of critical watershed parameters are provided. This tutorial is currently under development.
- 9. BASINS is used to view the flow and concentration time series at locations within the watershed. If additional data are desired such as gaging station data, for comparison BASINS can be modified by updating the mwprj file (Figure 3) so that data can be viewed alongside simulation results (Whelan et al., 2017e, 2017f, 2017g).
- 10. The SARA Timeseries Utility can be used to publish HSPF microbial densities at specified locations in a text (.txt) format for consumption by other components (Whelan et al., 2017h).
- 11. The MRA-IT consumes the text-based files to perform a risk assessment by estimating probabilities of infections from pathogens. This final step is not part of the QMRA set of tutorials since MRA-IT has its own tutorial (Soller et al., 2008).

A summary of characteristics associated with the QMRA functionality is presented in Table 1.

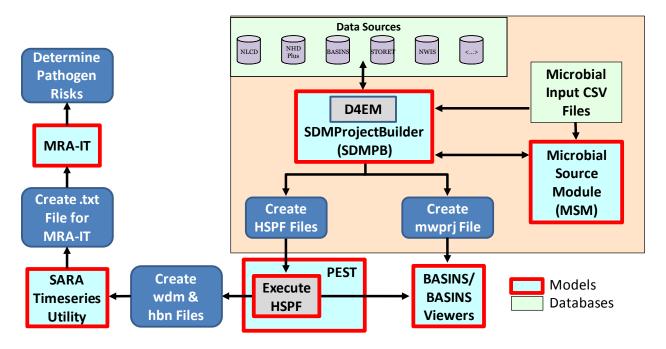


Figure 3. QMRA Workflow (After Whelan et al., 2014a)

Table 1. Summary of Characteristics associated with the QMRA modeling system

- Uses modeling tools and systems familiar to and used by the Office of Water such as HSPF and BASINS
- Focuses on watershed-based assessments
- Automates many data collection processes for watershed analysis
- Allows HUC-12 or Pour Point analyses
- Automates watershed delineation, accounting for minimum stream lengths, minimum subwatershed sizes and minimum land use type sizes
- Delineates the watershed into subwatersheds automatically at user-defined locations which usually account for sampling, monitoring, gaging, boundary condition locations, or locations for risk calculations.
- Provides a Microbial Properties Data within Local Data files that contain physico-microbial properties relevant to release, fate, transport, exposure, and effects modeling, where appropriate.
- Provides the option of using monitored or radar, remote sensing precipitation data
- Assigns NLDAS radar precipitation data automatically, when that option is selected, to individual subwatersheds when observed data are scarce, incorrect, or inappropriate (such as too far away).
- Processes manure-based source terms automatically to estimate manure/microbial loads on all subwatersheds, based on the number of animals correlated to land-use patterns, and automatically pre-populates input files of the models with these data.
- Processes manure-based point sources automatically, such as septic systems, WWTP or POTWs, on all subwatersheds and pre-populates input files of the models with these microbial data automatically.
- Automates pre-population of HSPF input-data requirements, accounting for
 - Snow accumulation/melt
 - Microbial fate and transport
 - o Different simulation time increments (e.g., hourly, daily, monthly, etc.).
- Is compatible with and uses functionality of HSPF
- Is compatible with and uses functionality of BASINS (e.g., viewers, both graphical and tabular)
- Allows manual manipulation of non-spatial, input data for more refined and boutique assessments
- Allows users to inspect and interrogate water flows and microbial concentration time series at multiple, user-defined locations throughout the watershed.
- Allows linkage to the pathogen risk model, MRA-IT

QMRA DOCUMENTATION

A series of tutorials and documents have been developed to aid users in implementing QMRA-related software. This section summarizes step-by-step instructions, through a series of tutorials and documents, that are available to the user for implementing a mixed-use, watershed-based QMRA, and suggests the order for reading and reviewing the tutorials. The tutorials begin with an explanation as where one obtains the modeling components and procedures for installing them. This is followed by tutorials and documents that describe how to execute the software at a site, beginning with relatively simple problems and progressively solving more complex ones. As one progresses through the tutorials, one will note that many of the steps repeat themselves, reinforcing the execution process as the problems become more complicated.

- 1. **Installation of Software for Watershed Modeling in Support of QMRA** This tutorial provides instructions on how to access, retrieve, download and install the following software (Whelan et al., 2017i):
 - a. SDMProjectBuilder (which includes the Microbial Source Module; Local data CSV files; SARA Timeseries Utility; and HSPF and PEST related calibration files for flow)^a
 - b. BASINS (which includes WinHSPF and WinHSPFlt)
 - c. SARA Timeseries Utility
 - d. FORTRAN Library
 - e. PEST
- Navigate the SDMPB and Identify an 8-digit HUC of Interest This tutorial reviews screens, icons and basic functions of the SDMProjectBuilder (SDMPB) that allow identification of an 8-digit HUC from which a pour point or 12-digit HUC can be chosen for a microbial assessment (Whelan et al., 2017d). It demonstrates how to
 - a. Identify and delineate an 8-digit HUC
 - b. Initiate the execution of SDMPB
 - c. Navigate the SDMPB
 - d. Use basic functions of the SDMPB tool bar
- 3. Import Microbial Property Data and Source Files to Identify and Modify Contamination Sources and Input Parameters (12 Default Local Data Files) This tutorial provides instructions and information on (Whelan et al., 2017a):
 - a. Identifying locations of point and non-point sources of contamination;
 - b. Providing guidance on modifying values of parameters that impact the release, migration, fate and transport of microbes within a watershed; and
 - c. Controlling delineation of a watershed into subwatersheds by identifying key locations that represent subwatershed boundaries.
- **4. Mathematical Formulations of the Microbial Source Module (MSM)** This document describes mathematical formulations that are the basis for the MSM (Whelan et al., 2017b). The MSM estimates microbial loading rates to land surfaces from non-point sources, and to streams from

^a The SDMPB also installs SWAT- and SWATCUP-related calibration files for flow, sediment, and nutrients. Although not microbial related, similar data are required for SWAT and HSPF, so the SDMPB was designed to also automatically populate SWAT's input files for flow, sediment, and nutrient watershed modeling. For additional information, refer to Kim et al. (2016a, 2016b).

point sources, for each subwatershed within a delineated watershed. A subwatershed which is the smallest modeling unit represents the common basis for information consumed and produced by the MSM. Non-point sources include numbers, locations, and shedding rates of domestic agricultural animals (dairy and beef cows, swine, poultry, etc.) and wildlife (deer, duck, raccoon, etc.). Monthly maximum microbial storage and accumulation rates on the land surface, adjusted for die-off, are computed over an entire season for four land-use types (cropland, pasture, forest and urbanized/mixed-use) for each subwatershed. Monthly point source microbial loadings to instream locations (i.e., stream segments that drain individual subwatersheds) are combined and determined for septic systems, direct instream shedding by cattle, and POTWs/WWTPs.

- 5. **Land-applied Microbial Loadings within a 12-Digit HUC** This tutorial reviews screens, icons, and basic functions of the SDMPB (Whelan et al., 2017e). It shows how to
 - a. Initiate execution of the SDMPB.
 - b. Navigate the SDMPB.
 - c. Identify and label a 12-digit HUC.
 - d. Consider land-applied waste, leaking septic systems, instream shedding by domestic animals, and shedding by domestic animals and wildlife to land surfaces
 - e. Develop necessary input files to execute HSPF successfully.
 - f. Develop necessary input files to view results from the SDMPB and HSPF.
 - g. Register the HSPF simulation with BASINS.
 - h. Use HSPF to simulate SDMPB's problem statement.
 - i. View simulation results of flows and microbial densities with BASINS.
- 6. Pour Point Analysis of Land-applied Microbial Loadings and Comparison of Simulated and Gaging Station Results This tutorial demonstrates a pour point analysis. It shows how to (Whelan et al., 2017f):
 - a. Initiate execution of the SDMPB.
 - b. Navigate the SDMPB.
 - c. Choose a pour point within a watershed, delineate the sub-area contributing to that pour point and collect data for it.
 - d. Consider land-applied waste, leaking septic systems, instream shedding by domestic animals, and shedding by domestic animals and wildlife to land surfaces
 - e. Develop necessary input files to execute HSPF.
 - f. Develop necessary input files to view results from the SDMPB and HSPF.
 - g. View simulation results for flows and microbial densities with BASINS.
 - h. Retrieve observed daily USGS flows and compare to simulated daily flows at the pour point.
- 7. Using NLDAS and NCDC Meteorological Data This tutorial reviews how screens, icons, and basic functions of the SDMPB use NLDAS data and land-based National Climatic Data Center (NCDC) weather (gauge) stations' MET data to support microbial fate and transport, in a watershed, by the HSPF watershed model (Whelan et al., 2017c). The application is performed using watersheds of different scales, including HUC-12 and pour-point delineations. A discussion of how to access and retrieve MET data from the National Oceanic and Atmospheric Administration's NCDC web site is also provided.

- 8. Point Source and Land-applied Microbial Loadings within a 12-Digit HUC This tutorial demonstrates importing and assessing a point source time series of microbial loadings, within a 12-digit HUC, by simulating microbial fate and transport with HSPF (Whelan et al., 2017g). It demonstrates how to
 - a. Initiate execution of the SDMPB.
 - b. Navigate the SDMPB.
 - c. Identify and label a 12-digit HUC.
 - d. Consider land-applied waste, leaking septic systems, instream shedding by domestic animals, and shedding by domestic animals and wildlife to land surfaces
 - e. Consider an instream point source loading of microbes.
 - f. Develop necessary input files to execute HSPF successfully.
 - g. Develop necessary input files to view results from the SDMPB and HSPF.
 - h. View simulation results for flows and microbial densities with BASINS.
- 9. Publishing a Microbial Density Time Series as a TXT File This tutorial reviews some of the screens, icons, and basic functions of the SARA Timeseries Utility tool, which allows users to publish HSPF data as a txt file (Whelan et al., 2017h). The SARA Timeseries Utility supports analysis and management of time-varying environmental data including listing, graphing, computing statistics, computing MET data, and saving in a WDM or text file. File formats supported include: WDM, HSPF Binary (.hbn), USGS RDB, and Text files (using the same import scripts as WDMUtil and BASINS). WDMUtil users will find that most of its functionality is included in this new utility.
- 10. HSPF Flow and Microbial Parameters Calibration with PEST This tutorial describes how to download and export flow observations and microbial densities from a watershed of interest with BASINS, prepare PEST input files for HSPF flow and microbial parameter calibrations, and perform HSPF flow and microbial parameter calibrations with PEST (Kim et al., 2017a).
- 11. Supplemental Notes: Isolated Subwatersheds and Binary Printing This tutorial provides supplemental notes to address issues associated with the QMRA infrastructure, including isolated subwatersheds and binary printing. Isolated subwatersheds occur when the delineation process results in subwatersheds that are not connected to the water body network of the larger watershed. This tutorial describes how the user can manually connect the isolated subwatershed to the rest of the watershed (Kim et al., 2017b). In addition, printing to binary files during the calibration process can result in a large amount of data being generated and printed to files, resulting in longer calibration run times. This document describes the options for printing data to binary files.

DISCLAIMER

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