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Quantitative Microbial Risk Assessment Tutorial

Installation of Software for Watershed Modeling in Support of QMRA

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Summary

This tutorial provides instructions for accessing, retrieving, and downloading the following software to install on a host computer in support of Quantitative Microbial Risk Assessment (QMRA) modeling:

- QMRA Installation
- SDMProjectBuilder (which includes the Microbial Source Module; microbial property data and source files; HSPF- and PEST-related calibration files for flow and microbes; SARA Timeseries Utility; and SWAT and SWATCUP related calibration files for flow, sediment, and nutrients)
- BASINS (which includes WinHSPF and WinHSPFlt)
- SARA Timeseries Utility
- FORTRAN Library
- PEST

Installation of Software for Watershed Modeling in Support of QMRA

PURPOSE

Summarize the software required for implementing a Quantitative Microbial Risk Assessment (QMRA).

OBJECTIVE

Provide instructions for accessing, retrieving, downloading, and installing software on a host computer in support of Quantitative Microbial Risk Assessment modeling.

DEMONSTRATION

This tutorial provides instructions on how to retrieve, download, and install the following software:

- QMRA Installation Package, which includes documents, tutorials, and SDMProjectBuilder setup files.
- SDMProjectBuilder, which installs the following components:
    - Microbial Source Module, which determines initial microbial loading rates
    - HSPF- and PEST-related calibration files for flow and microbes
    - Microbial Property Data and Source Files, which capture user-defined microbial loading source terms and locations, and provides the POTW discharge time series for a Point Source example
    - SARA Timeseries Utility, which saves an executable that converts output formats, and provides an example concentration time series that supports a tutorial for publishing a microbial density time Series as a TXT File.
    - SWAT and SWATCUP related calibration files for flow, sediment, and nutrients:
- BASINS, which provides a user-friendly interface for HSPF and whose download includes a Windows version of HSPF with a user-friendly interface, and a “lite” version of HSPF used for batch simulations for model calibration
- SARA Timeseries Utility, which creates a shortcut icon for the “SARA Timeseries Utility” executable on the user’s computer screen that saves text output as UTF-8, omits the Byte Order Marker at the beginning of the file, skips the title line in the file if the title is blank, and skips the date column if all date and time components are hidden
- FORTRAN Library, which is an executable used to properly execute PEST input files for HSPF parameter calibration
- PEST, which is an inverse model for calibrating model parameters to observations

Users should execute installation instructions on only those software products that have

- not been previously installed or
- been previously installed, but require an updated version.

If software was installed using an installation package (e.g., InstallShield Setup Wizard), then the software should be removed using the Microsoft Windows Add/Remove feature. If files (e.g., zip files) are just downloaded from a web site to the host computer, then these files can be removed manually. If software does NOT need to be installed, skip to the appropriate point in the installation instructions.

Note that the example folder structures are only examples; as such, and the examples provided in the different sections of this tutorial may not necessarily be consistent. For example, one download may suggest C:\SDMPB\, while another may suggest C:\Users\gwhelan\iemTechnologies\SDMPB\. Regardless, just be consistent with your downloads.

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REFERENCES

APPENDIX A: Example Folder Structure when Implementing a Site Assessment using the SDMProjectPuilder

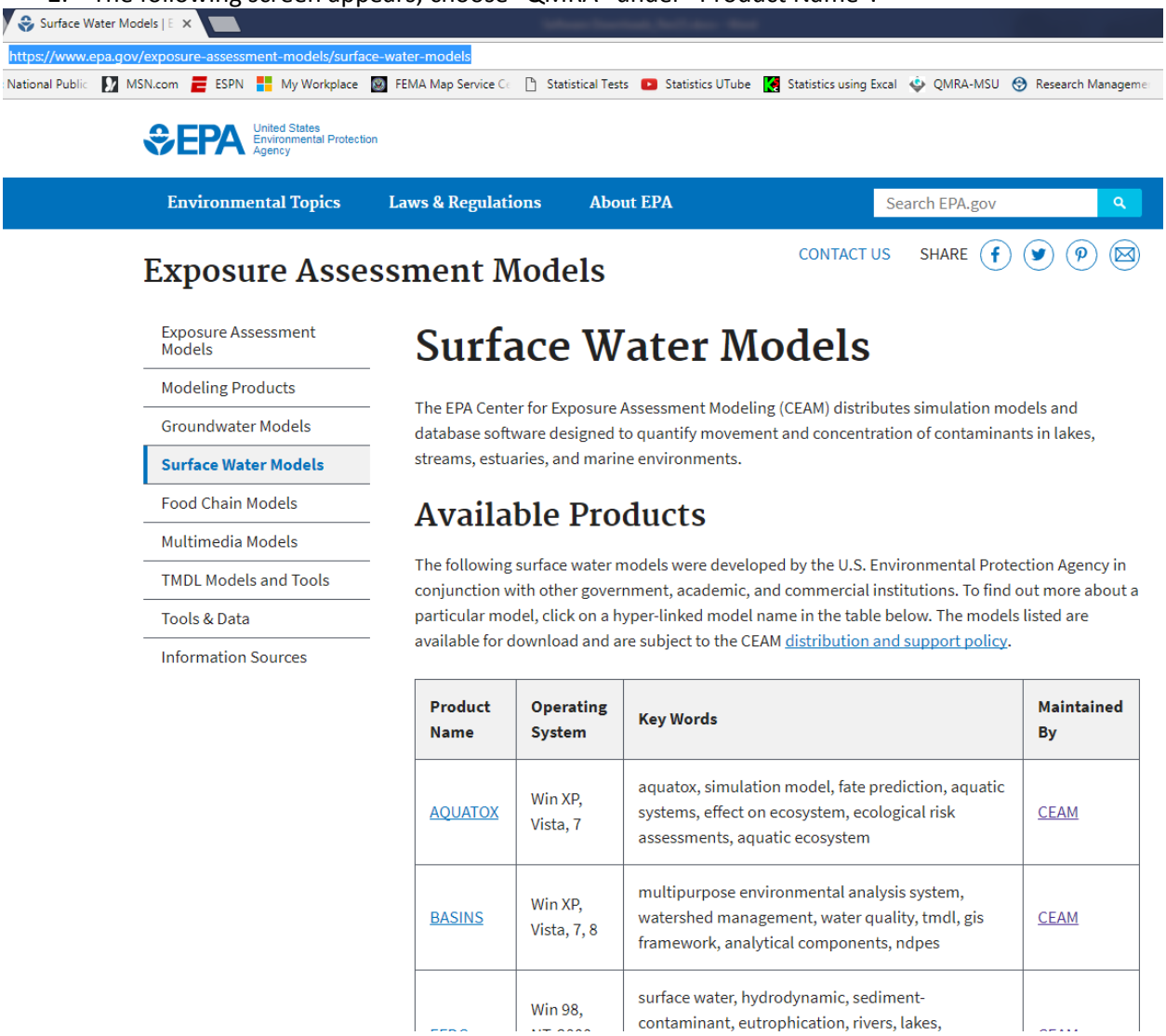
QMRA Installation Package

If the user has already downloaded the "QMRA_Installation_Package.zip" file, then skip this section. The steps to download the "QMRA_Installation_Package.zip" file are as follows.

1. Access the following U.S. Environmental Protection (EPA) Center for Exposure Assessment Modeling (CEAM) web site under Surface Water Models.

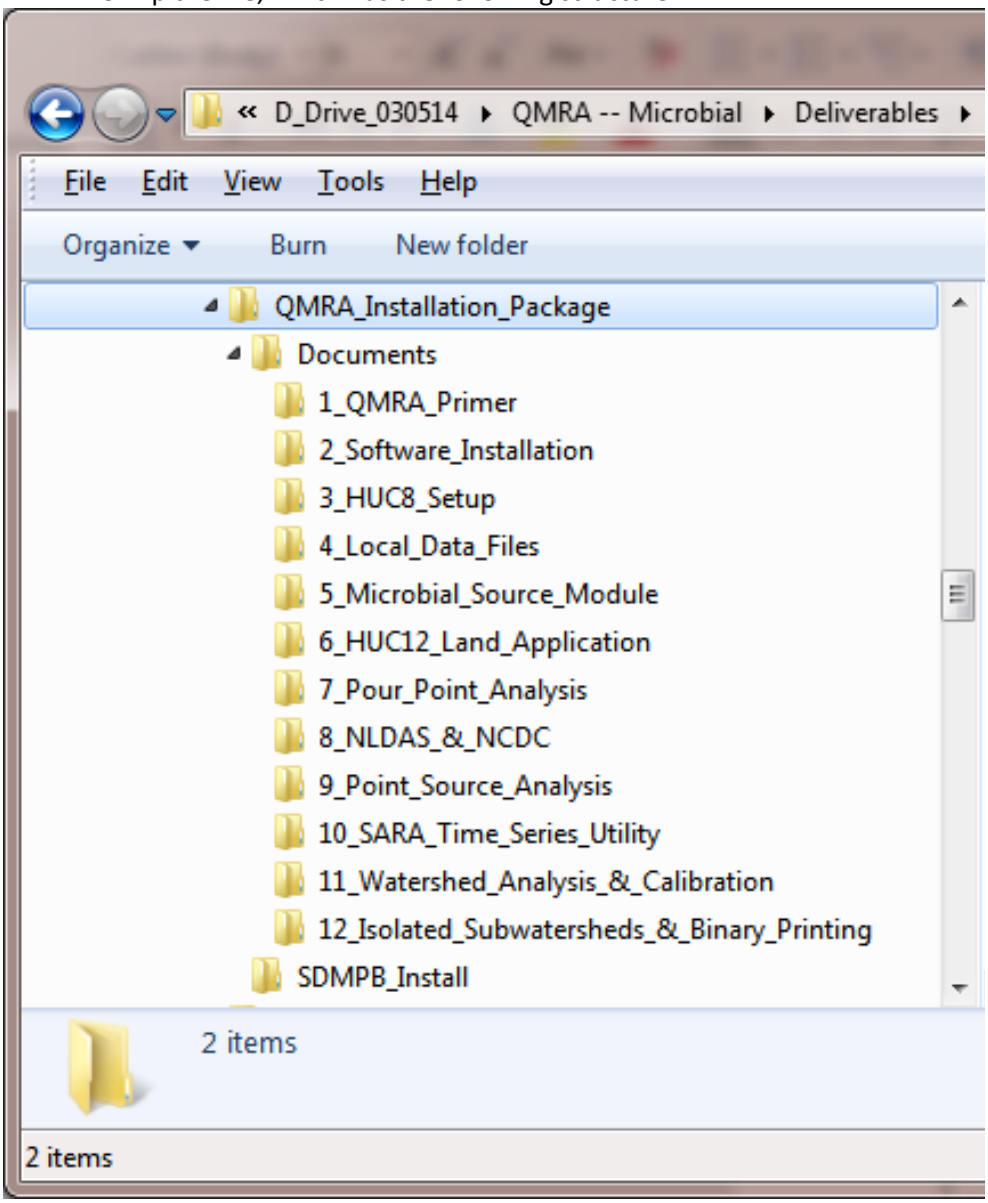
https://www.epa.gov/exposure-assessment-models/surface-water-models

2. The following screen appears; choose "QMRA" under "Product Name".



3. Download “QMRA_Installation_Package.zip” to a folder where the user has administration privileges, *such as your user’s folder (*e.g., *C:\Users\<your name>).*

4. Unzip the file, which has the following structure.



The QMRA installation package is a zip file (“QMRA_Installation_Package.zip”) that contain a folder, titled QMRA_Installation_Package, with two subfolders:

- Documents -- contains 12 informational documents and tutorials, including this document, that have been developed to aid users in implementing QMRA-related software
- SDMPB_Install – contains the setup executable for installing the SDMProjectBuilder

DOCUMENTS

These documents should be reviewed in the following order:

1. **Primer –** This document 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 (Whelan et al., 2017a)
2. **Installation of Software for Watershed Modeling in Support of QMRA** – This tutorial provides instructions on how to access, retrieve, download and install software supporting the QMRA infrastructure (Whelan et al., 2017b):
3. **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., 2017c).
4. **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., 2017d) identifying locations of point and non-point sources of contamination; providing guidance on modifying values of parameters that impact the release, migration, fate and transport of microbes within a watershed; and controlling delineation of a watershed into subwatersheds by identifying key locations that represent subwatershed boundaries.
5. **Mathematical Formulations of the Microbial Source Module (MSM) –** This document describes mathematical formulations that are the basis for the MSM (Whelan et al., 2017e). The MSM estimates microbial loading rates to land surfaces from non-point sources, and to streams from point sources, for each subwatershed within a delineated watershed.
6. **Land-applied Microbial Loadings within a 12-Digit HUC** – This tutorial reviews screens, icons, and basic functions of the SDMPB for performing a microbial assessment on a 12-Digit HUC (Whelan et al., 2017f).
7. **Pour Point Analysis of Land-applied Microbial Loadings and Comparison of Simulated and Gaging Station Results** – This tutorial demonstrates a microbial assessment on a watershed delineated based on a user-specified pour point (Whelan et al., 2017g).
8. **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., 2017h).
9. **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., 2017i).
10. **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., 2017j).
11. **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).
12. **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.

SDMProjectBuilder

The SDMProjectBuilder installation is located in the folder <…*installation folder*\SDMPB Install\> and includes two files:

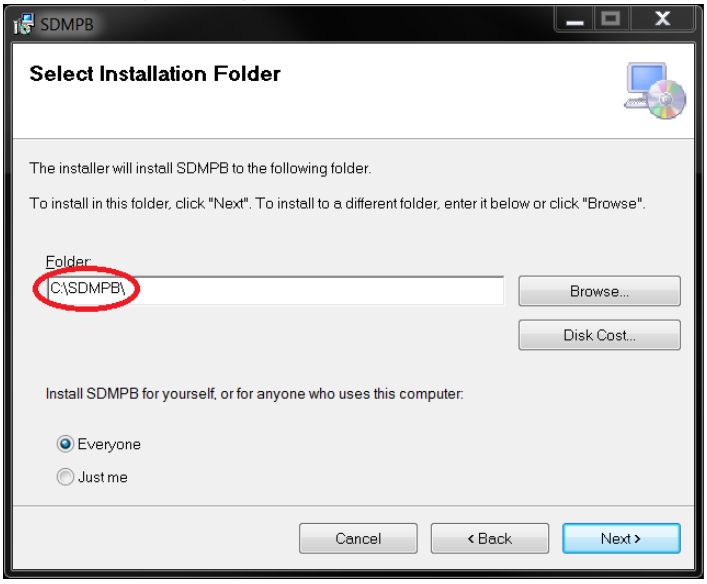
- **InstallSDMPB.msi**, which is used for installation, storage, and removal of programs
- **Setup.exe**, which installs the SDMProjectBuilder.exe, a desktop icon, and related files

The installation is initiated when "Setup.exe" is executed.

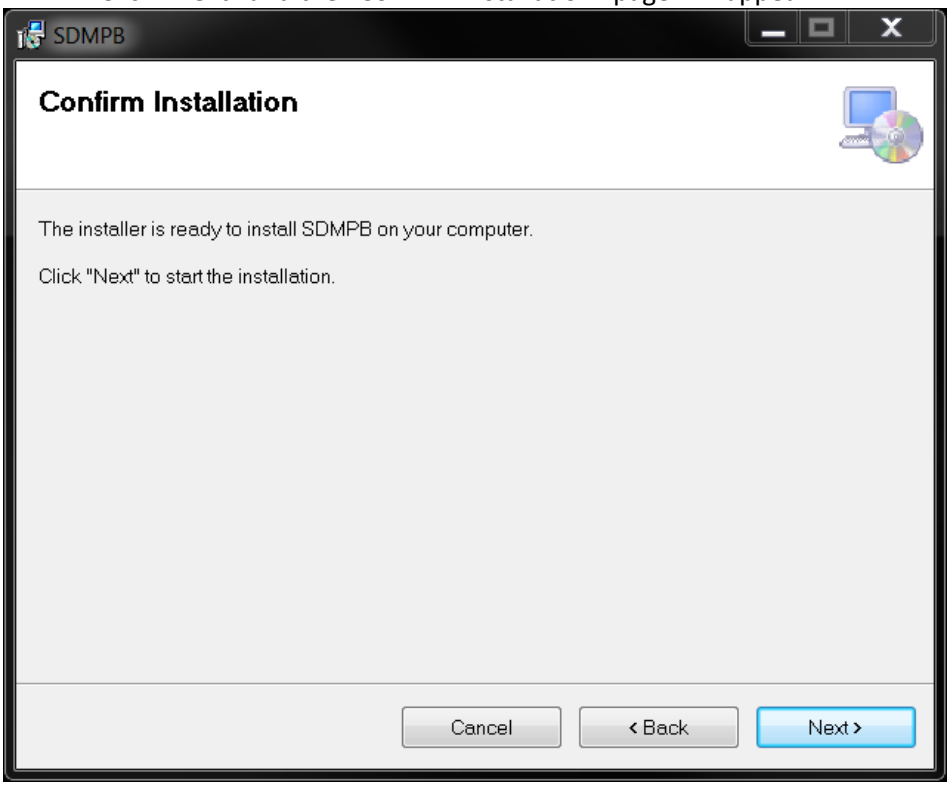
1. After downloading, run Setup.exe, and follow the installation instructions.

2. A Setup window will appear.

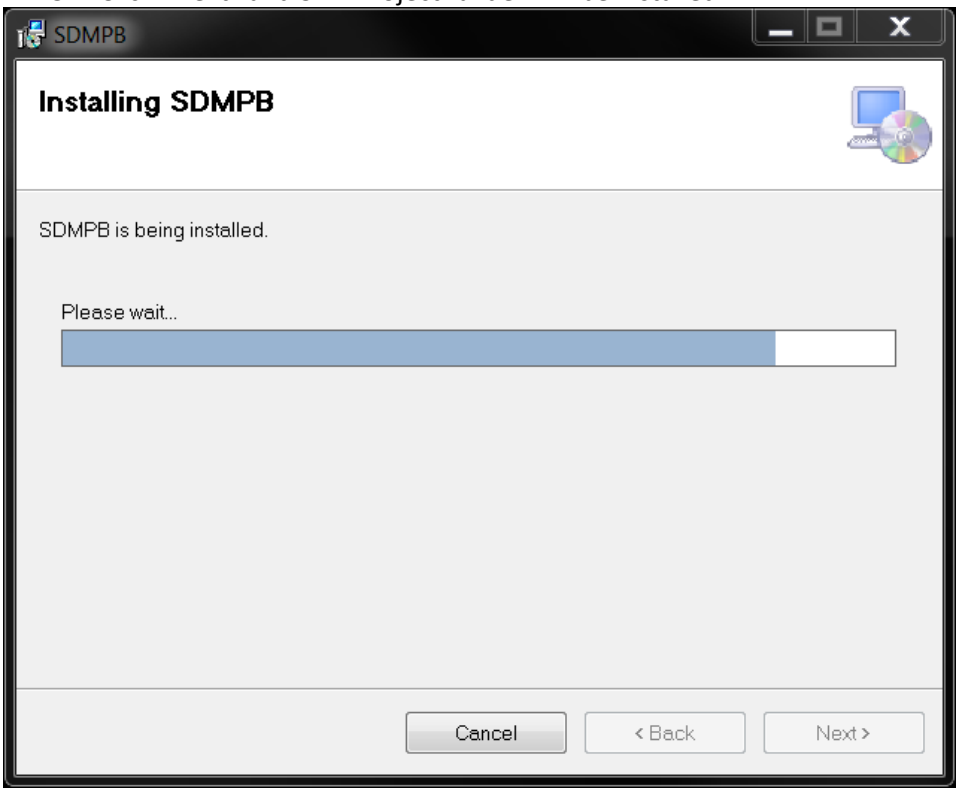
3. Click "Next", and the "Select Installation Folder" window will appear. Select the folder path with administrative privileges where you will install SDMProjectBuilder, such as the user's folder (C:\Users\<your name>). In the example below, SDMProjectBuilder will be installed in "C:\SDMPB\".



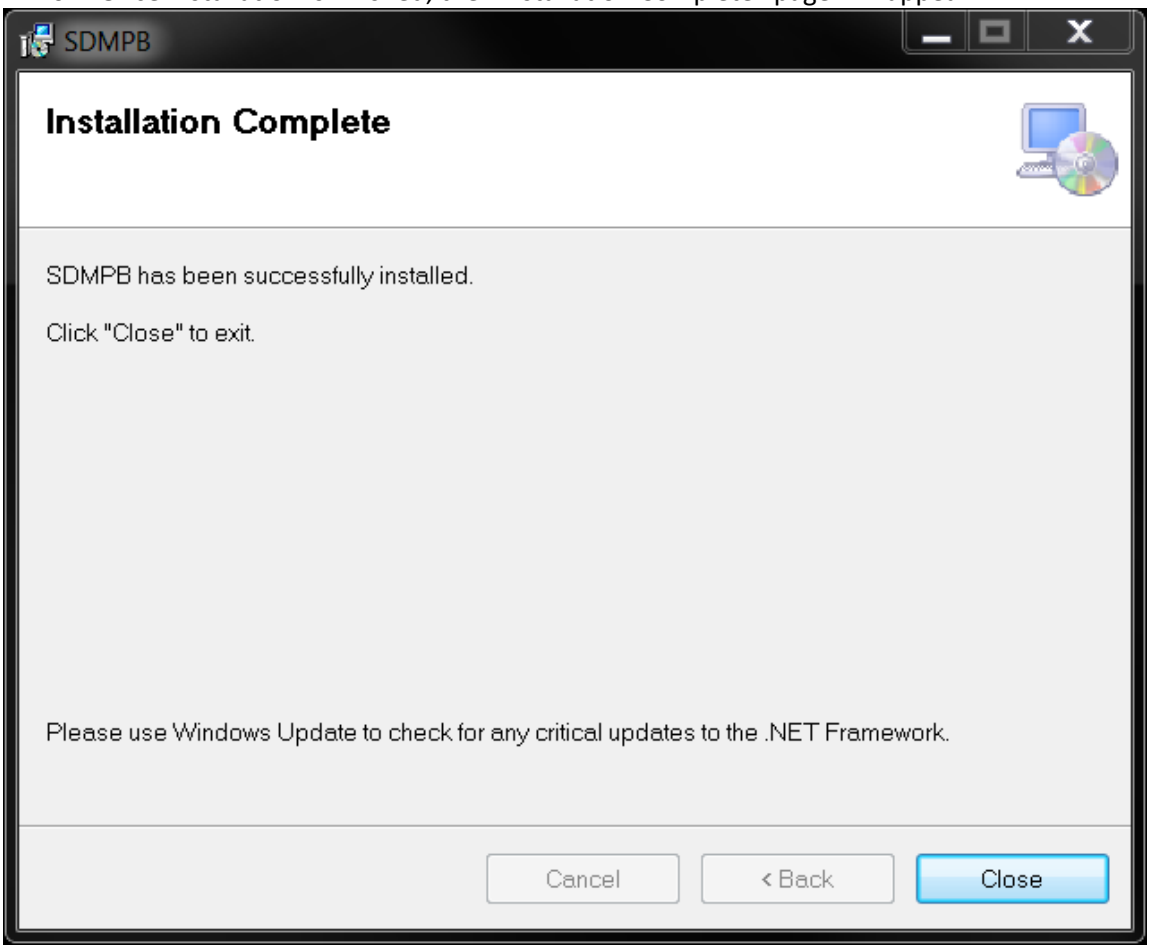
4. Click “Next” and the “Confirm Installation” page will appear.



5. Click “Next” and SDMProjectBuilder will be installed.



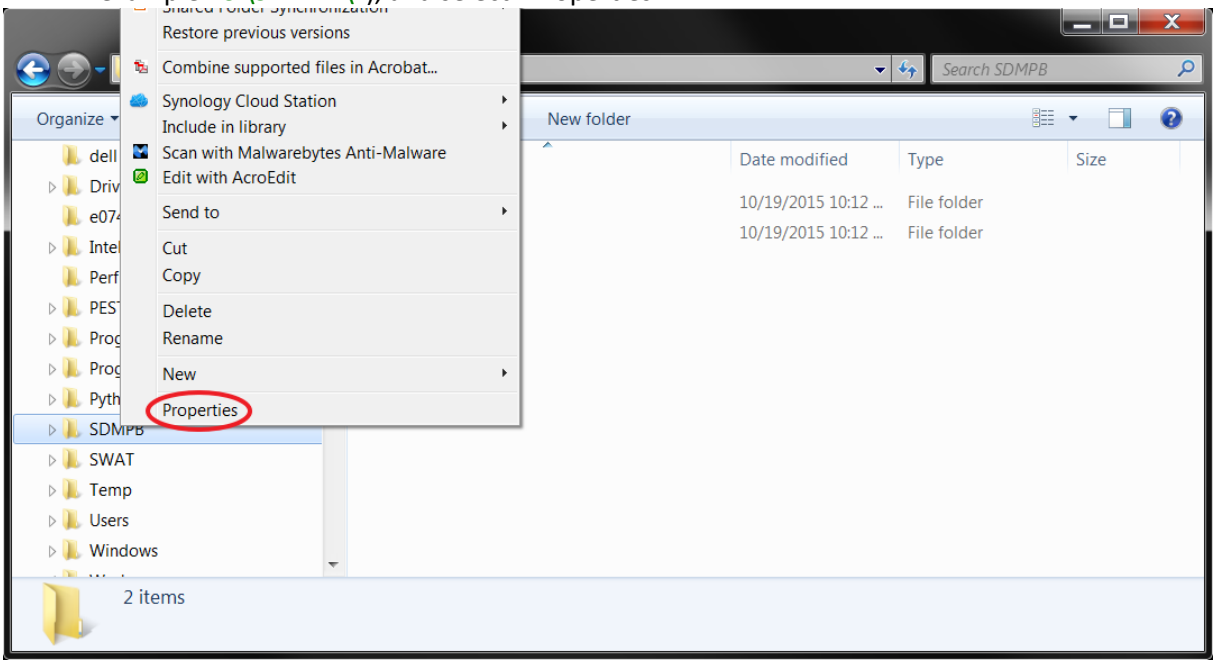
6. Once installation is finished, the “Installation Complete” page will appear.



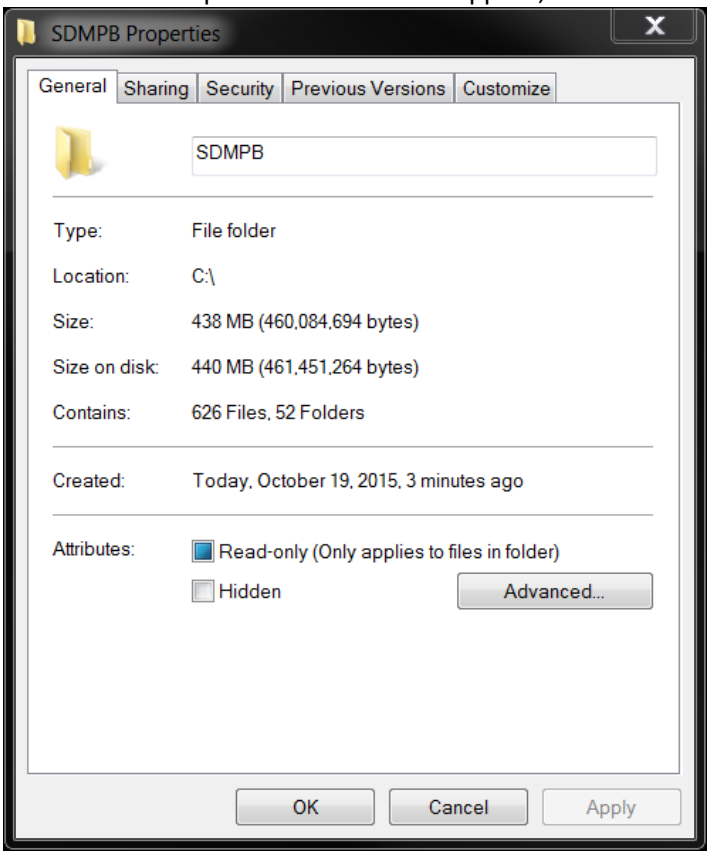
7. Click “Close”, and you will now find a shortcut icon for SDMProjectBuilder on your computer’s Desktop.

8. If the shortcut icon cannot be found on the Desktop screen, locate the executables on the hard drive (i.e., SDMProjectBuilder.exe), typically in the folder labeled \SDMPB\bin\.

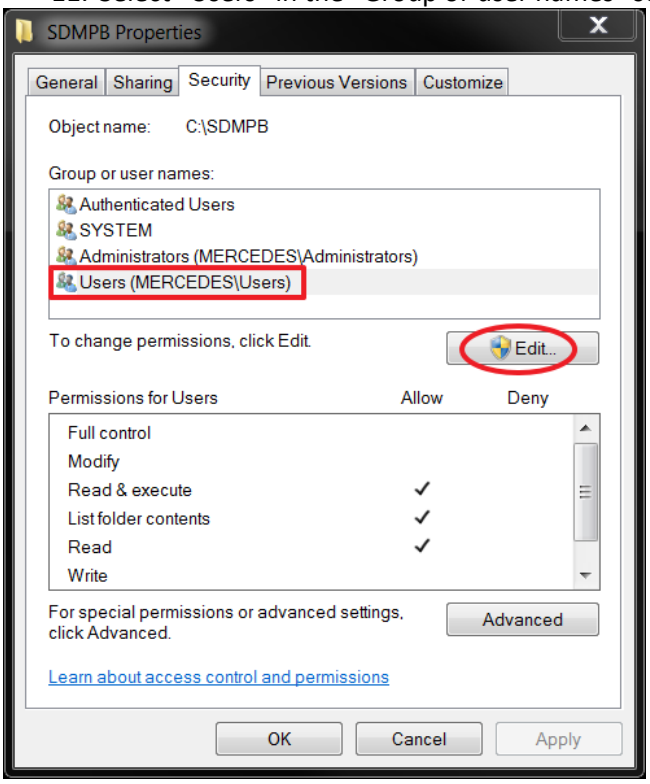
9. The user will need to have “Full control” on the folder where SDMProjectBuilder is installed. To confirm user control, right-click on the folder where SDMProjectBuilder was installed (in this example “C:\SDMPB\”), and select “Properties”.



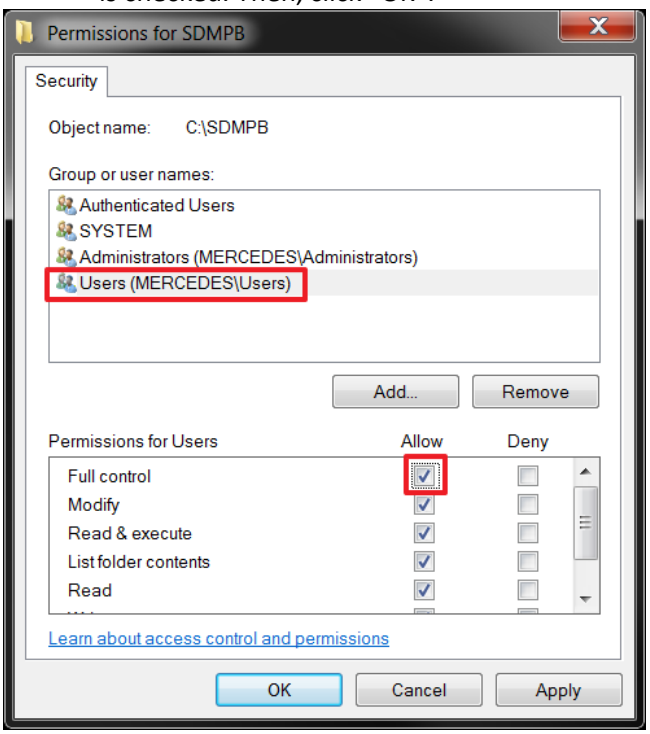
10. The “Properties” window will appear, and select the “Security” tab.



11. Select “Users” in the “Group or user names” section, and click “Edit”.



12. The “Permissions” for SDMPB folder will appear. In the window, select “Users” in “Group or user names” section, and ensure “Allow” for “Full control” under the “Permissions for Users” section is checked. Then, click “OK”.



Following Setup.exe execution, the following key files are created:

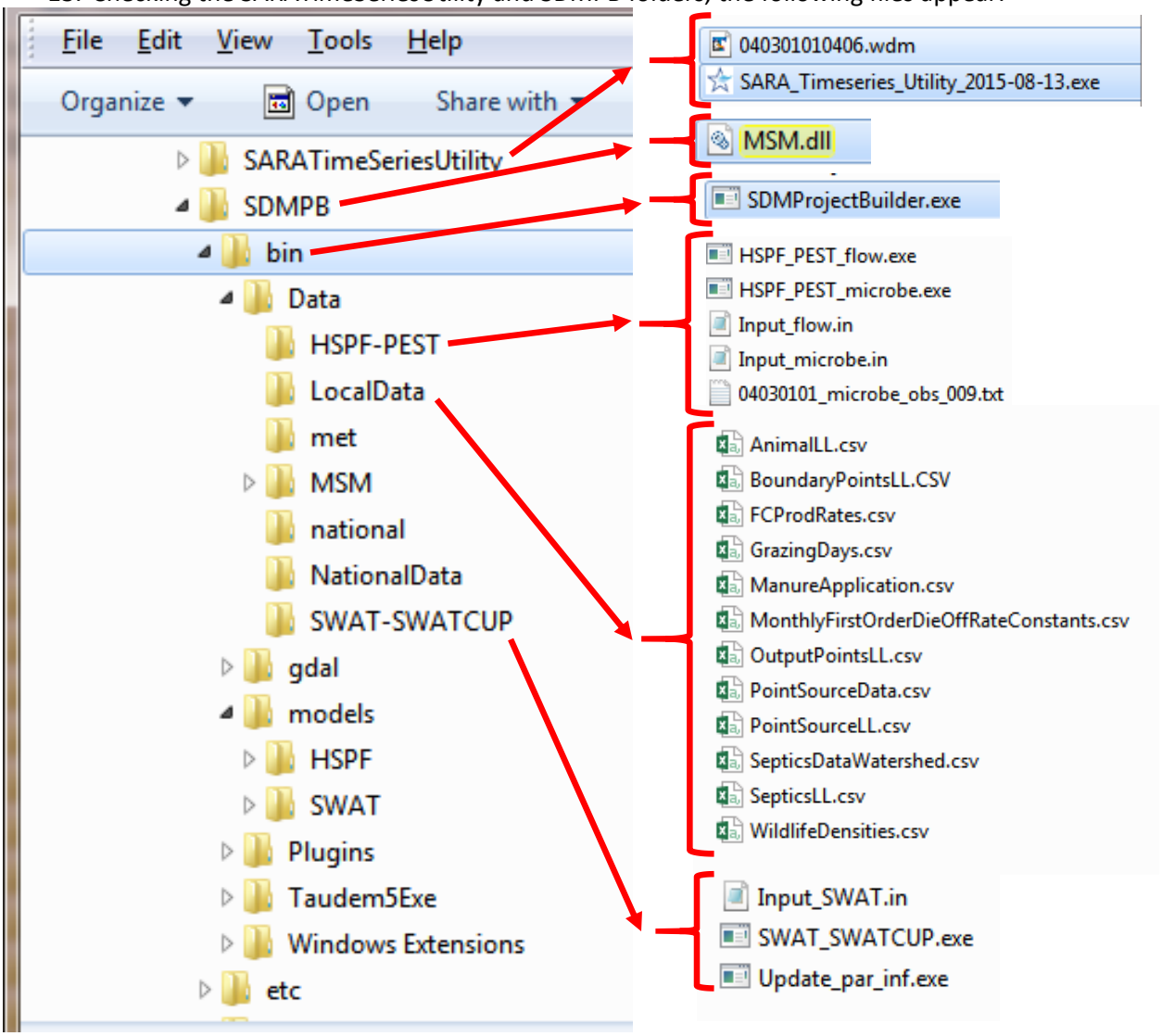
- SDMProjectBuilder Executable (SDMProjectBuilder.exe), which is executed for each unique site-specific assessment
- Microbial Source Module (MSM.dll) for determining initial microbial loading rates
- HSPF and PEST related calibration files for flow and microbes
    - Input_flow.in, which is an example input file containing the flow parameters used in the HSPF calibration process, as well as default input files that contain folder locations of HspfLt [batch (or light) version of HSPF], observed data used in the calibration, and PEST
    - HSPF_PEST_flow.exe, executable compiled with FORTRAN that prepares the inverse model PEST input files for HSPF flow parameter calibrations
    - Input_microbe.in, which is an example input file containing the microbial parameters used in the HSPF calibration process, as well as default input files that contain folder locations of HspfLt [batch (or light) version of HSPF], observed data used in the calibration, and PEST
    - HSPF_PEST_microbe.exe, executable compiled with FORTRAN that prepares the inverse model PEST input files for HSPF microbial parameter calibrations
    - 04030101_microbe_obs_009.txt, which is a file that contains observed microbial densities (i.e., concentrations) at a sampling location [e.g., near the outfall (i.e., mouth)] of the watershed; these data are used in the microbial calibration tutorial.
- Microbial Property Data and Source Files:
    - 12 Local Data CSV files, which capture user-defined microbial properties, and microbial loading source terms and locations
    - "POTW Point Source Example.xlsx", which provides the POTW discharge time series for a Point Source example
- SARA Timeseries Utility:
    - Time_Series_Utility_2015-08-13.exe, which saves an executable that converts output formats, and provides an example concentration time series that supports a tutorial for publishing a microbial density time Series as a TXT File.
    - 040301010406.wdm, used to demonstrate how a concentration time series is converted to a txt file
- SWAT and SWATCUP related calibration files for flow, sediment, and nutrients:
    - SWAT_SWATCUP.exe, which is a SWAT-CUP input file generator used in the SWAT calibration process
    - Input_SWAT.in, which is a default input file of "SWAT_SWATCUP.exe"
    - Update_par_inf.exe, which updates and provides the new ranges of parameters after each SWAT-CUP iteration during the calibration process

Users should place these files in a folder where they have administrative privileges. These files represent the base files for any site assessment or applications of tutorials. When executing a site assessment (i.e., SDMProjectBuilder.exe), a unique site-specific working folder is created and only the 1) HSPF and PEST related calibration files for flow and microbes and 2) Local Data CSV files are automatically copied to the working folder, as these are the only files that may be unique to that specific microbial assessment. An example folder structure is presented in Appendix A.

The two flow calibration files ("HSPF_PEST_flow.exe" and "Input_flow.in") **MUST** always be in the same folder. Likewise, "HSPF_PEST_microbe.exe", "Input_microbe.in", and "04030101_microbe_obs.txt" **MUST** always be in the same folder, although not necessarily in the same folder as the two flow calibration files.

The SWAT and SWATCUP are not necessary or used when performing microbial assessments. Likewise, the Local Data CSV files, HSPF, and PEST are not necessary or used when performing nutrient assessments using SWAT.

13. Checking the SARATimeSeriesUtility and SDMPB folders, the following files appear:



BASINS, WinHSPF3.0, and WinHSPFlt

If BASINS, WinHSPF3.0, and WinHSPFlt have already been downloaded to the computer, skip this step; otherwise, proceed with the installation. The BASINS installation package includes both forms of the HSPF model: WinHSPF3.0, the Windows version with a user-friendly, user interface; and WinHSPFlt, which is the "lite" version of HSPF used for batch simulations for model calibration. The version of BASINS being used with this workflow is one that has **NOT** been released through the BASINS 4.1 download web site (i.e., http://water.epa.gov/scitech/datait/models/basins/download.cfm) at this time. Instead, BASINS 4.5 will be used with this workflow.

1. A copy of the BASINS installer can be found on Dropbox and can be accessed at the following location, which includes a beta version of BASINS (version 4.5) with the latest updates and represents the version that should be used with these tutorials:

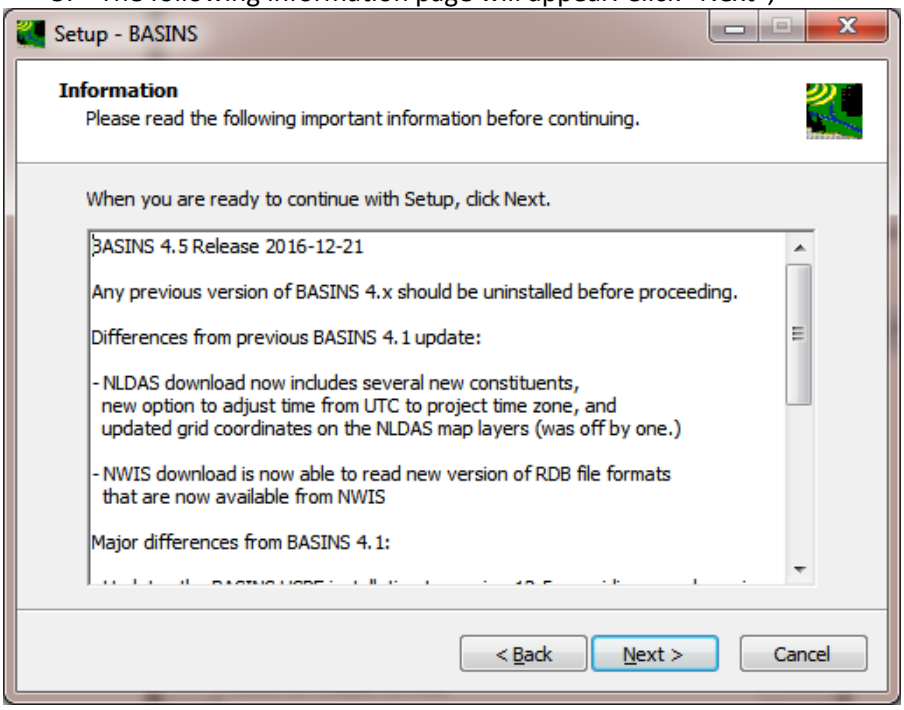
https://www.dropbox.com/s/k3vl7wnmp1i2ka1/BASINS4.5.2016.12.21Rev.exe?dl=0

2. Save the file, "BASINS4.5.2016.12.21Rev.exe", to the user's folder of choice. "BASINS4.5.2016.12.21.exe" contains the InstallShield installation executable.

3. Un-install any version of existing BASINS and HSPF software already installed.

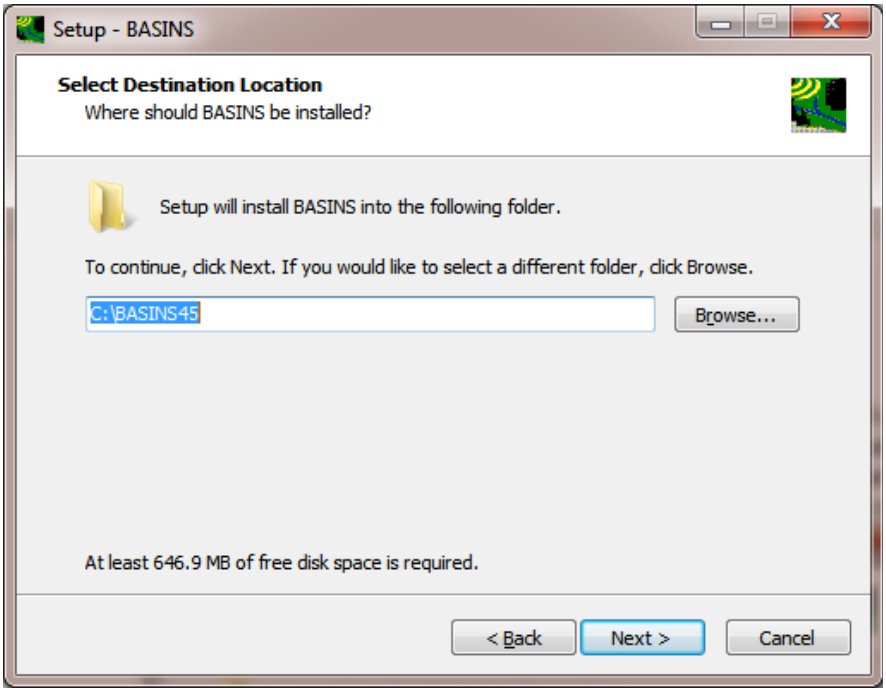
4. If you are the Administrator of your computer, execute "BASINS4.5.2016.12.21Rev.exe". The following setup window will appear. Click "Next".

5. The following information page will appear. Click “Next”,

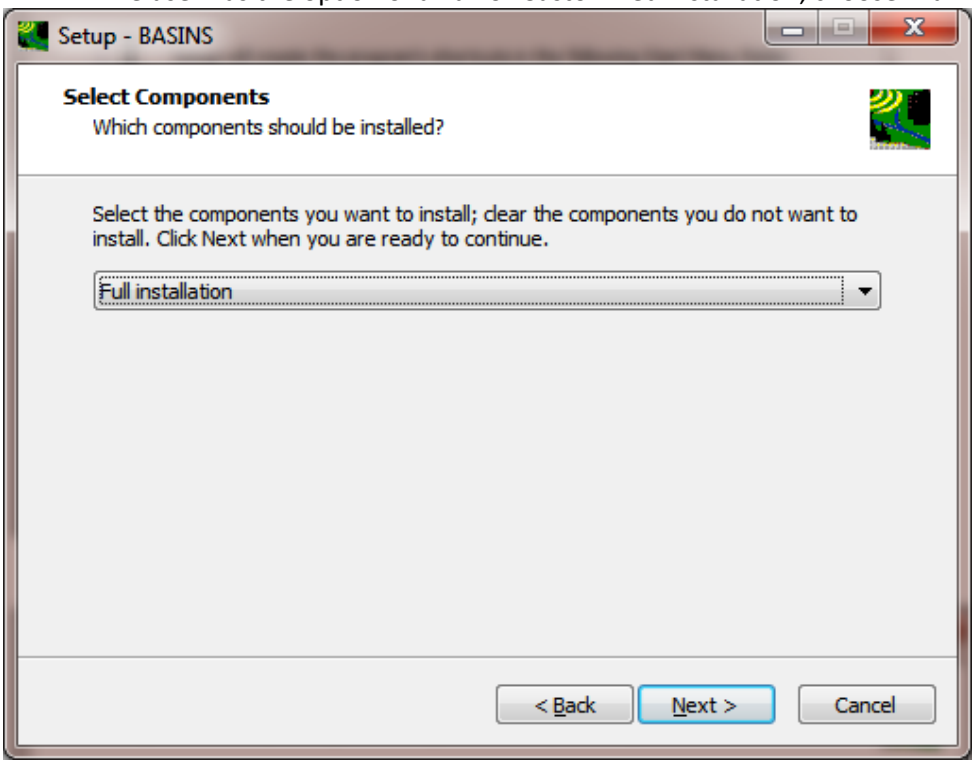


With the current version of the BASINS/HSPF software, we have found that using a different folder location could create execution problems with HSPF, so use the default director suggested by the installation software.

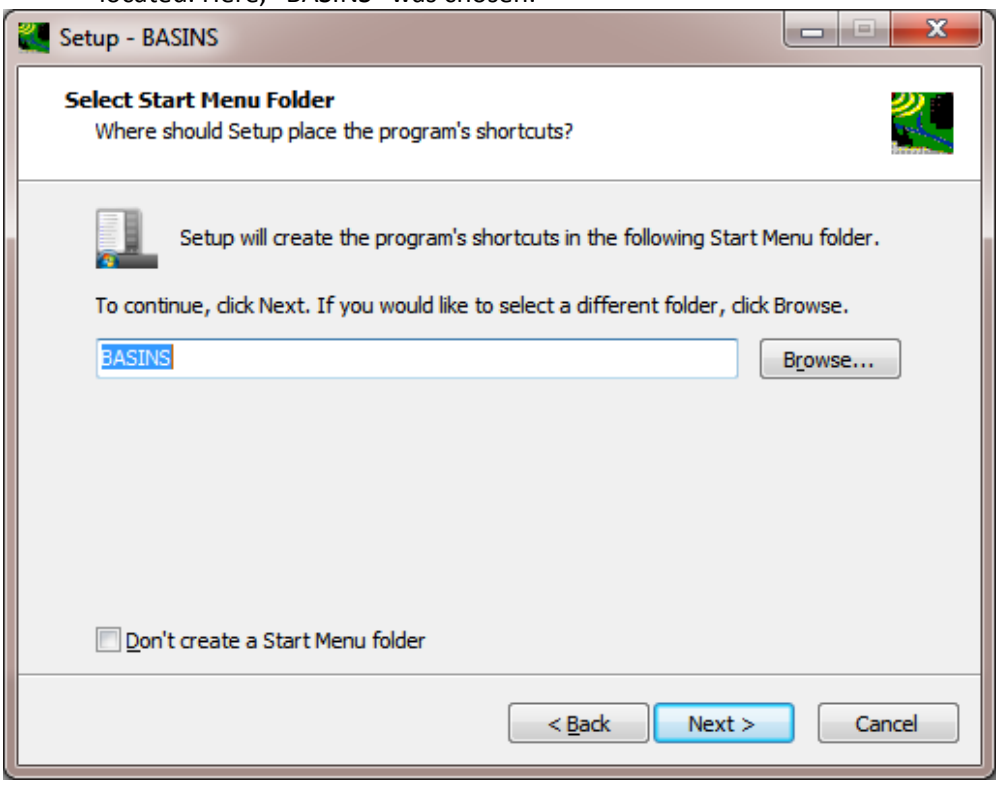
6. The “Select Destination Location” window will appear. Do not change the suggested folder location. Click “Next”.



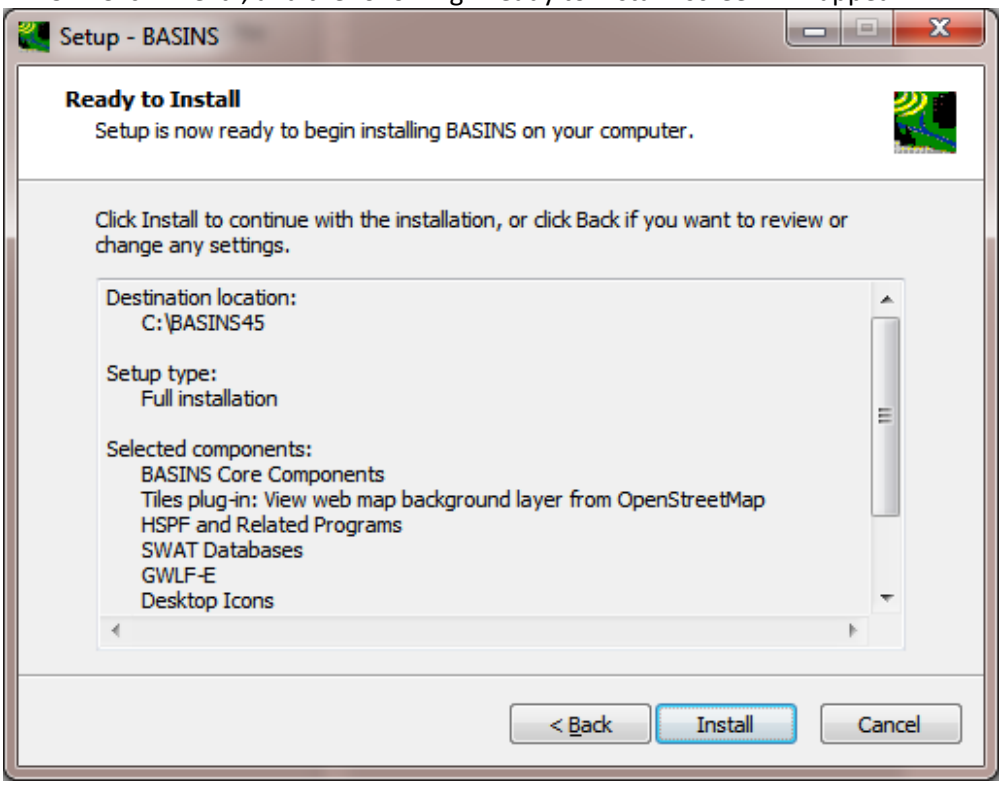
7. The user has the option of a Full or Customized installation; choose “Full installation”.



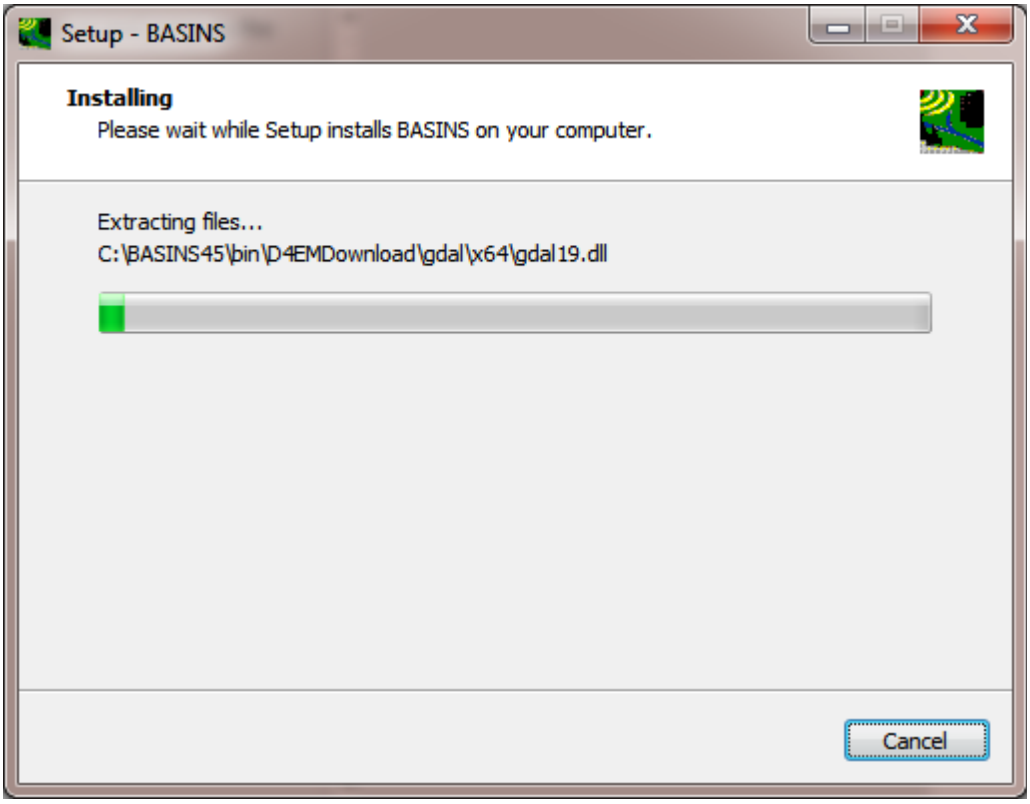
8. Click “Next”, and you can specify a Start menu folder where the program’s shortcuts will be located. Here,” BASINS” was chosen.



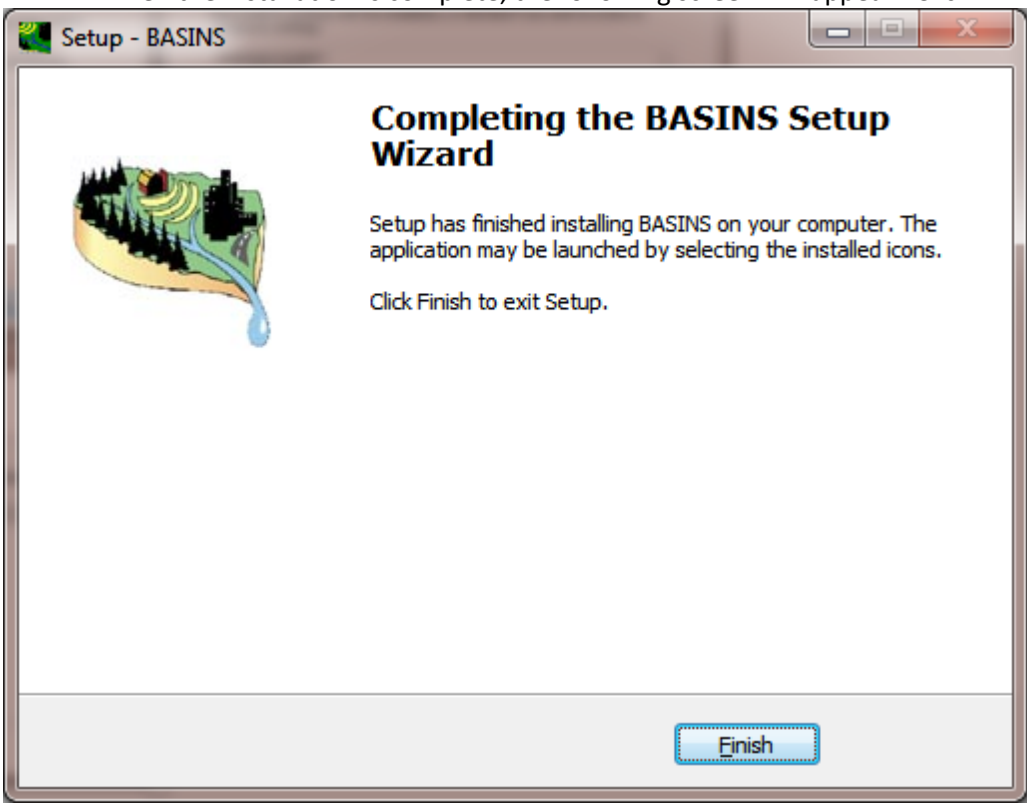
9. Click “Next”, and the following “Ready to Install” screen will appear:



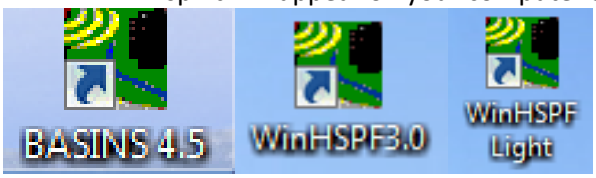
10. Click “Install”. BASINS will be installed with HSPF.



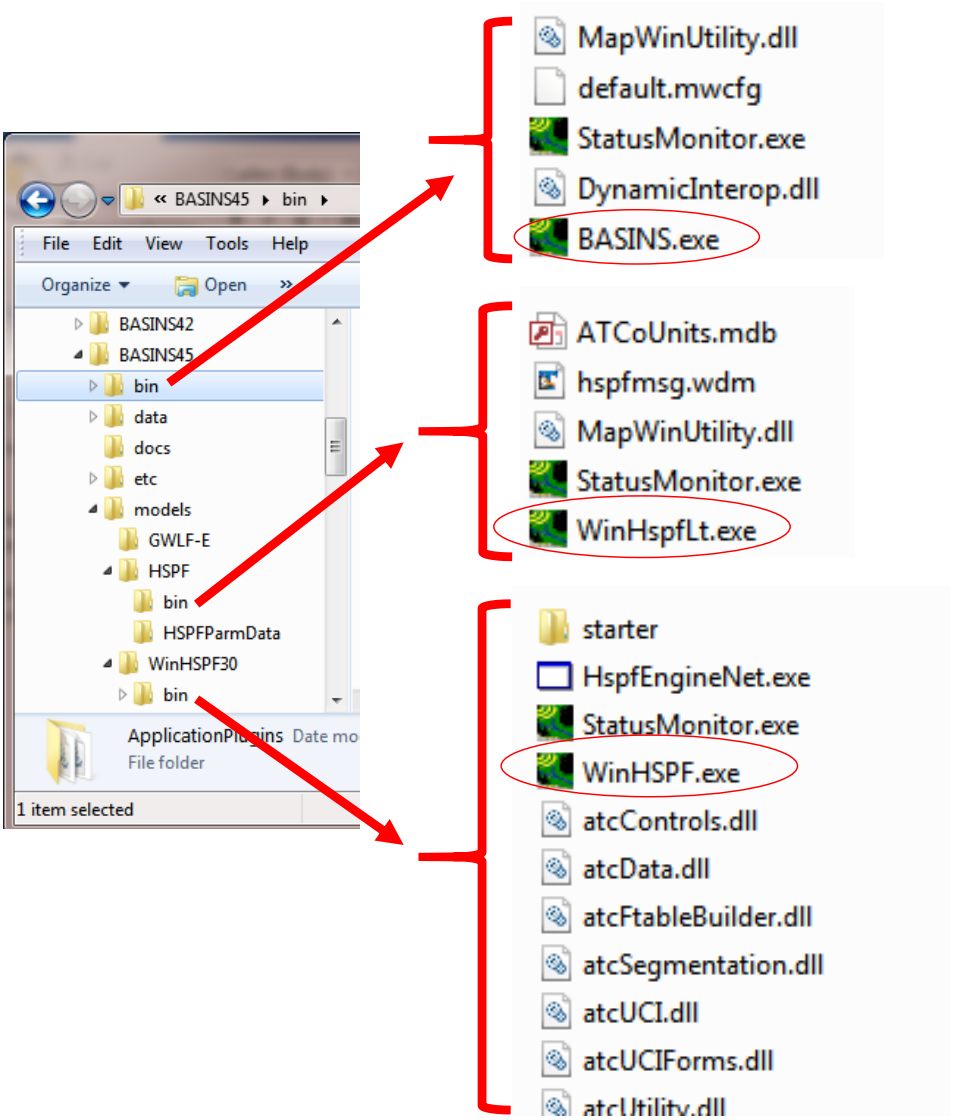
11. When the installation is complete, the following screen will appear. Click “Finish”.



12. Once the BASINS installation is finished, shortcut icons for BASINS 4.5, WinHSPF3.0, and WinHspfLt will appear on your computer’s Desktop.

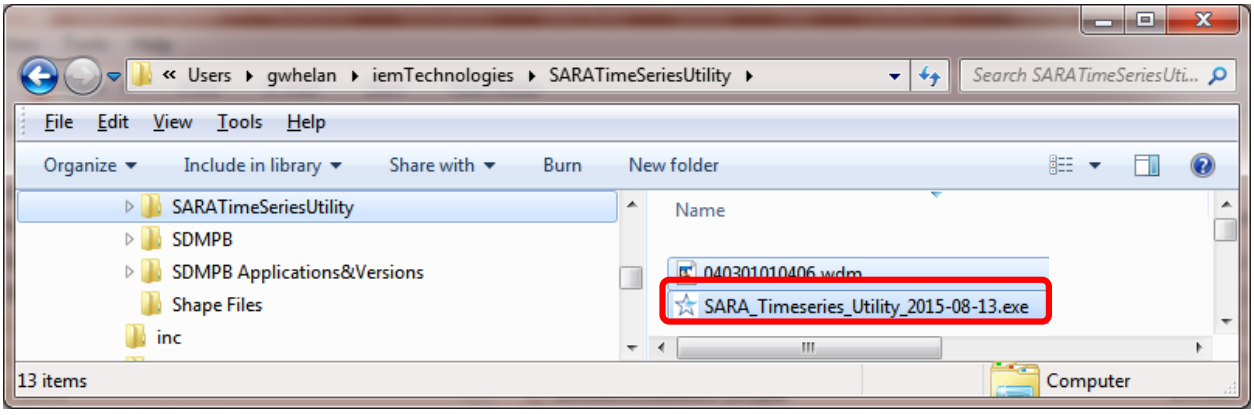


13. WinHSPF3.0 can run HSPF only through a user interface. WinHspfLt is a “lite” version of WinHSPF3.0 and can run HSPF on a Command window (e.g., batch runs). WinHspfLt is frequently coupled with other software such as PEST, FRAMES, etc. If the icons do not appear on the Desktop, locate the following executables – BASINS.exe, WinHspfLt.exe, and WinHSPF.exe – on the hard drive, where they are typically found in “\BASINS45\bin”, \BASINS45\models\HSPF\bin”, and “\BASINS45\models\WinHSPF30\bin”, respectively.


« BASINS45 ▸ bin ▸
File Edit View Tools Help
Organize Open
BASINS42
BASINS45
bin
data
docs
etc
models
GWLF-E
HSPF
bin
HSPFParmData
WinHSPF30
bin
File folder
1 item selected
MapWinUtility.dll
default.mwcfg
StatusMonitor.exe
DynamicInterop.dll
BASINS.exe
ATCoUnits.mdb
hspfmsg.wdm
MapWinUtility.dll
StatusMonitor.exe
WinHspfLt.exe
starter
HspfEngineNet.exe
StatusMonitor.exe
WinHSPF.exe
atcControls.dll
atcData.dll
atcFtableBuilder.dll
atcSegmentation.dll
atcUCI.dll
atcUCIForms.dll

SARA Timeseries Utility

1. Run the installer titled “SARA Timeseries Utility_2015-08-13.exe” by double-clicking on it from the folder



2. Running the installer as an Administrator may be required, depending on security settings and the chosen installation location. Place it in the file location you created earlier. A Shortcut icon for “SARA Timeseries Utility” (representing the executable “SARA Timeseries Utility.exe”) should now be on your computer screen:

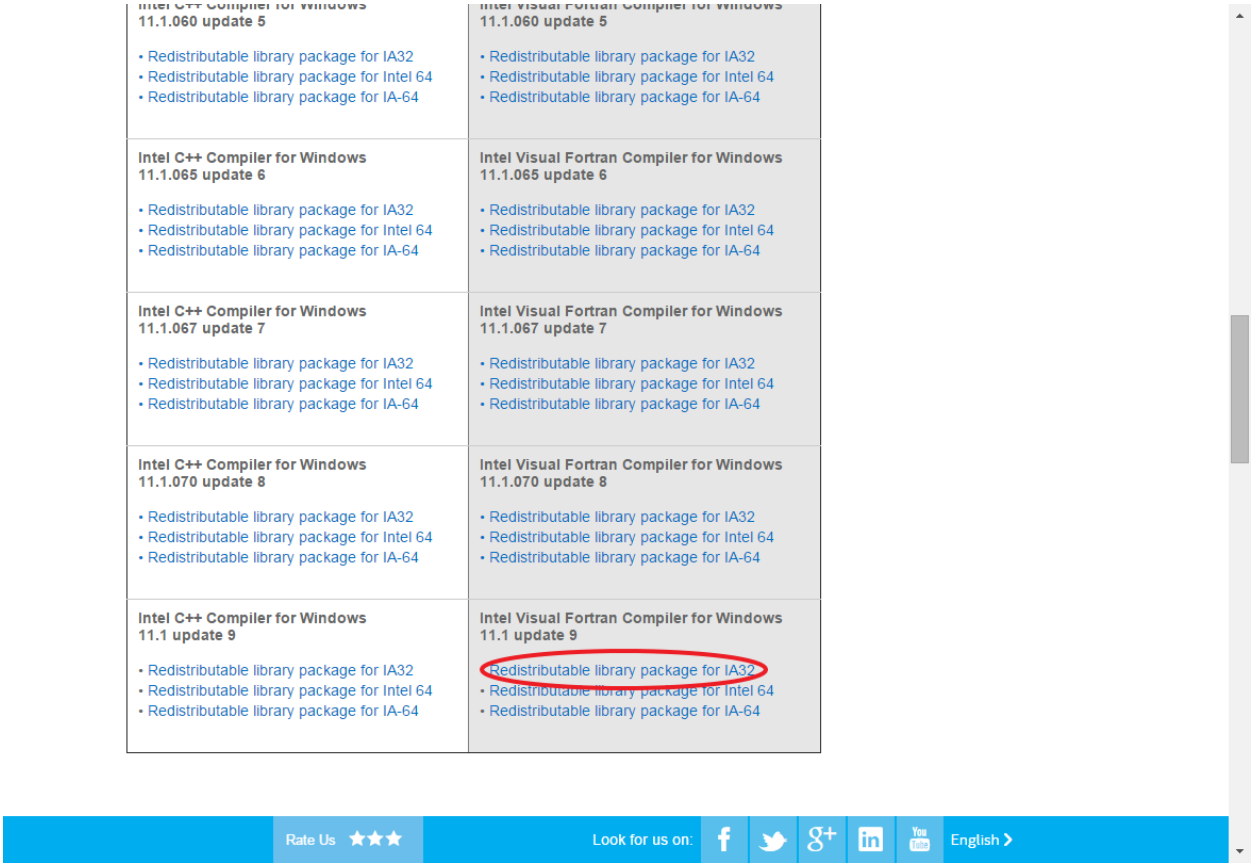
The “SARA Timeseries Utility.exe” saves text output as UTF-8, omits the Byte Order Marker at the beginning of the file, skips the title line in the file if the title is blank, and skips the date column if all date and time components are hidden.

FORTRAN Library

To properly execute PEST input files for HSPF parameter calibration which is an executable, the appropriate FORTRAN Library must be on the user's machine: "Intel® Visual Fortran Redistributables on IA-32". If this software already exists on the machine, skip this install; otherwise, proceed with this download to install.

1. Go to https://software.intel.com/en-us/articles/redistributable-libraries-of-the-intel-c-and-fortran-compiler-for-windows

2. Under "Links to the redistribution packages", download "Intel Visual Fortran Compiler for Windows 11.1 update 9 Redistribution library package for IA32" by clicking on "Redistribution library package for IA32".

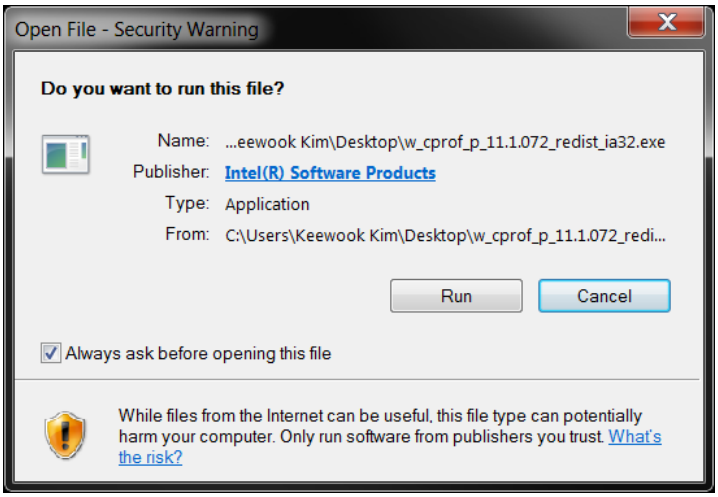


3. Select a folder where you have administrative privileges. In this example, the folder was

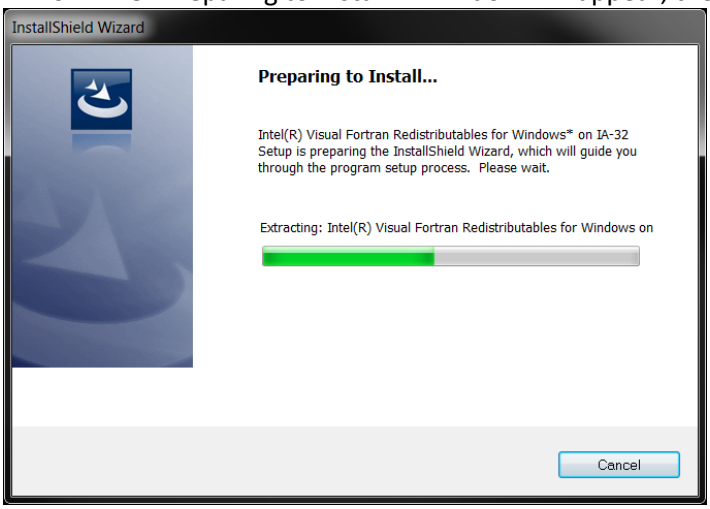
C:\Users\gwhelan\DLL download\Library Package IA32\

4. Execute "w_cprof_p_11.1.072_redist_ia32.exe".

5. An "Open File – Security Warning" window may appear. If so, click "Run", and a screen similar to the following may appear.

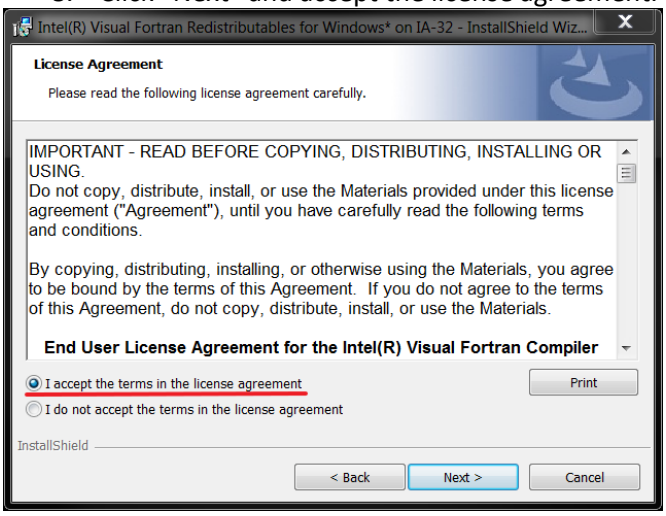


6. The “Preparing to Install…” window will appear, then disappear.

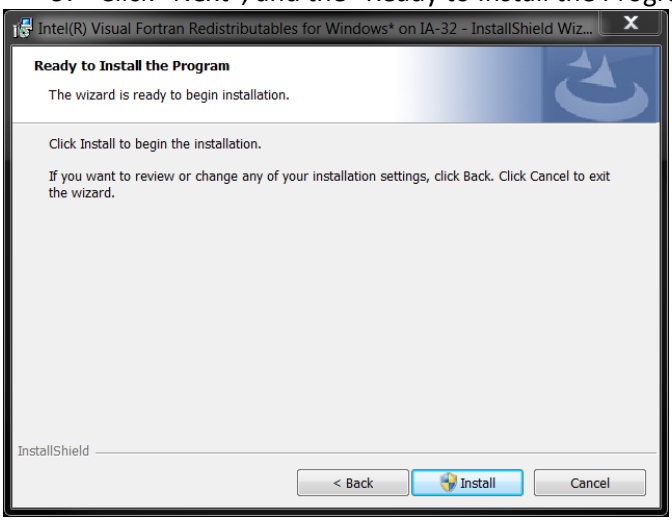


7. The InstallShield window will appear.

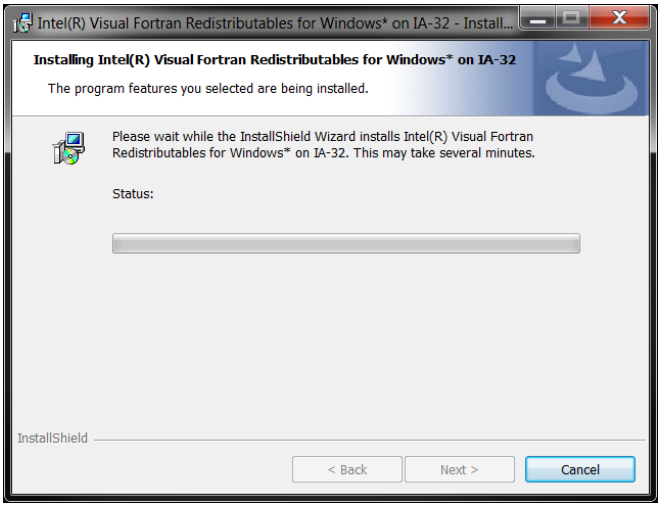
8. Click “Next” and accept the license agreement.



9. Click “Next”, and the “Ready to Install the Program” screen will appear.

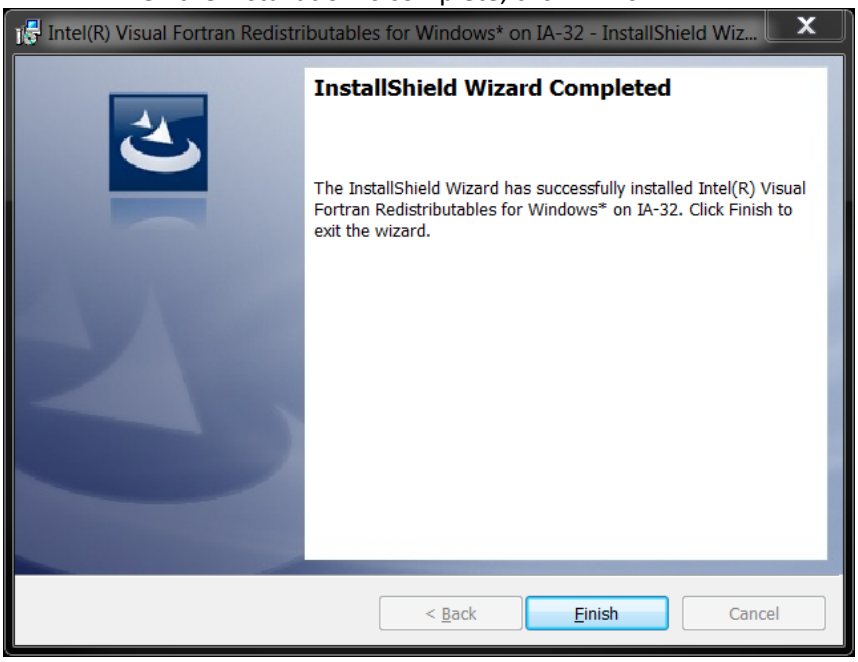


10. Click “Install”.



11. If “User Account Control” window appears during the installation, click “OK”.

12. When the installation is complete, click “Finish”.



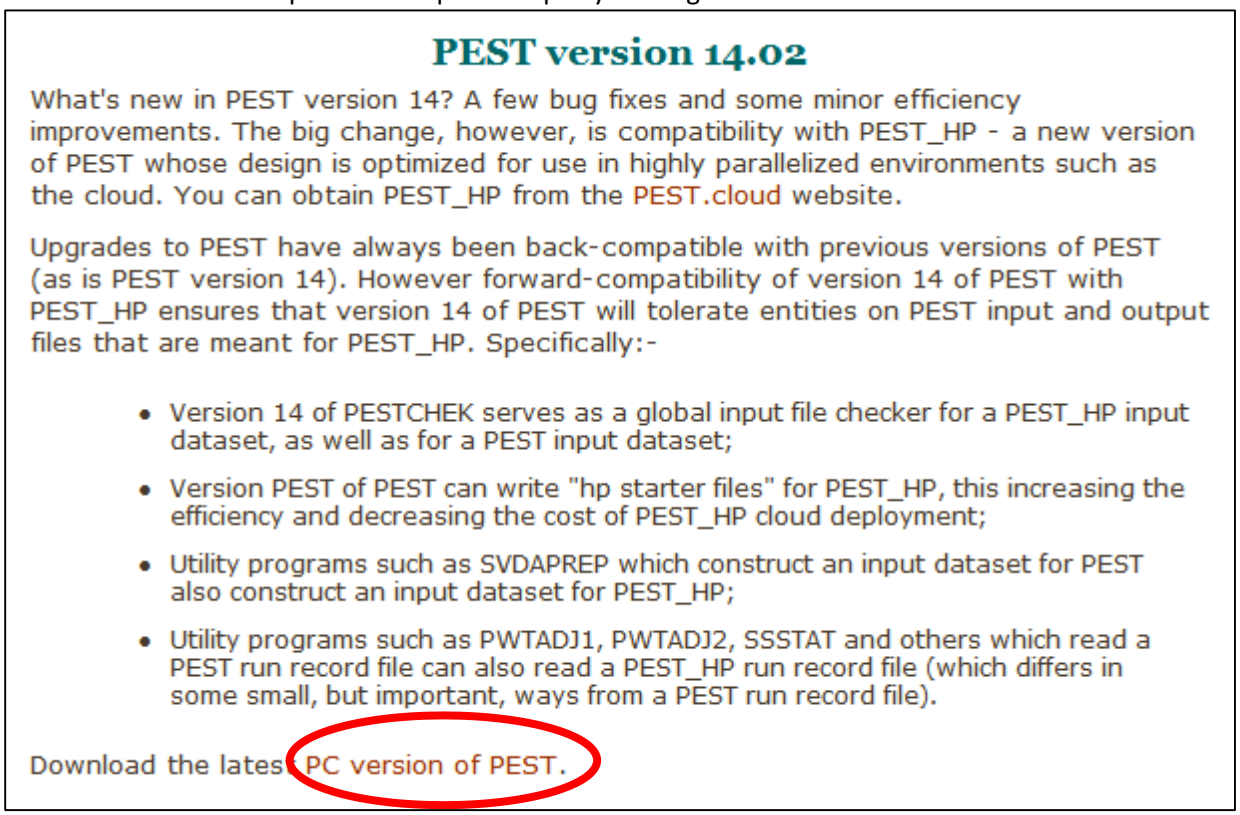
13. The FORTRAN Library is now on your machine.

PEST

Installation Procedure

If the user has already downloaded the latest version of PEST to the computer, skip this step; otherwise, proceed with the installation.

1. Go to http://www.pesthomepage.org/Downloads.php, and under "PEST version 14.2", download the zip file titled "pest14.zip" by clicking "PC version of PEST".



PEST version 14.02

What's new in PEST version 14? A few bug fixes and some minor efficiency improvements. The big change, however, is compatibility with PEST_HP - a new version of PEST whose design is optimized for use in highly parallelized environments such as the cloud. You can obtain PEST_HP from the PEST.cloud website.

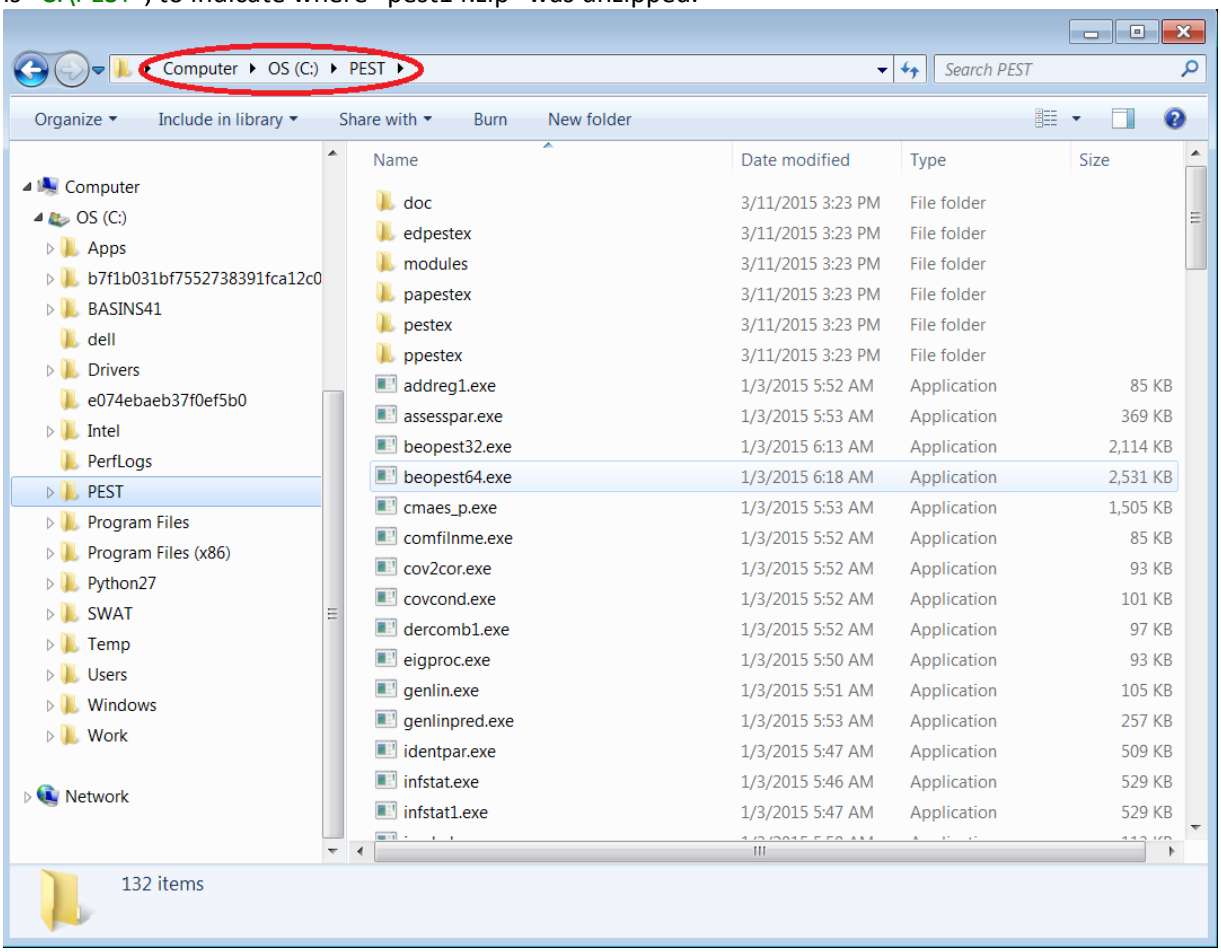
Upgrades to PEST have always been back-compatible with previous versions of PEST (as is PEST version 14). However forward-compatibility of version 14 of PEST with PEST_HP ensures that version 14 of PEST will tolerate entities on PEST input and output files that are meant for PEST_HP. Specifically:-

- Version 14 of PESTCHEK serves as a global input file checker for a PEST_HP input dataset, as well as for a PEST input dataset;
- Version PEST of PEST can write "hp starter files" for PEST_HP, this increasing the efficiency and decreasing the cost of PEST_HP cloud deployment;
- Utility programs such as SVDAPREP which construct an input dataset for PEST also construct an input dataset for PEST_HP;
- Utility programs such as PWTADJ1, PWTADJ2, SSSTAT and others which read a PEST run record file can also read a PEST_HP run record file (which differs in some small, but important, ways from a PEST run record file).

Download the latest PC version of PEST.

2. Unzip "pest14.zip" to a folder where you have administrative privileges, such as your user's folder (C:\Users\<your name>).

In the example below, a folder named “PEST” was created on the C: drive, so the full folder extension is “C:\PEST”, to indicate where “pest14.zip” was unzipped.



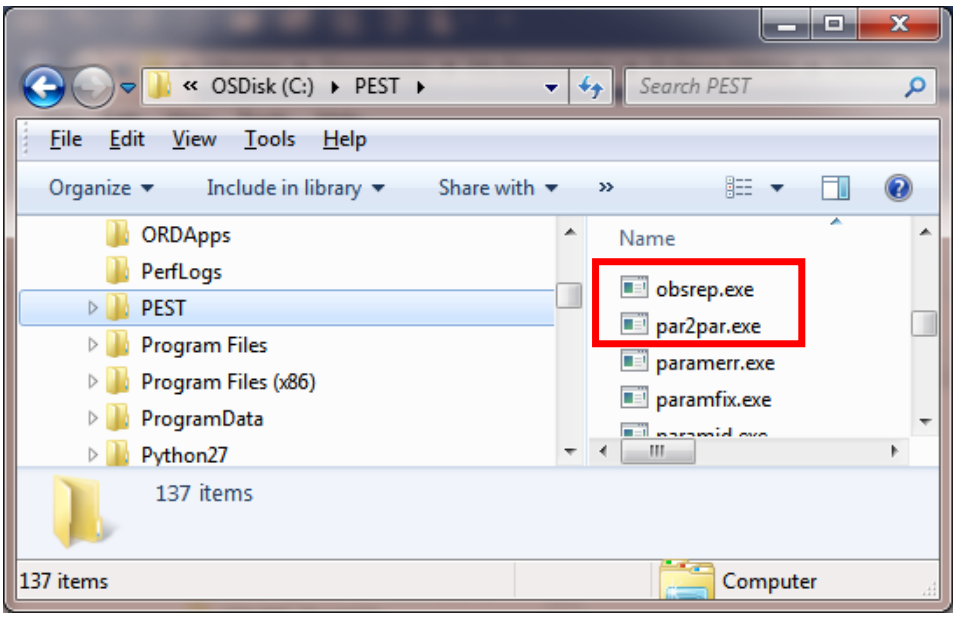
There is no required installation process for PEST. The user can copy “pest.exe” from the folder where “pest14.zip” was unzipped and place it in a folder where the user can run “pest.exe” in a Windows Command Window. The PEST manual (“postman.pdf”) can be found in the “doc” folder (see above figure). Running PEST separately will not be necessary, as an executable has been developed (HSPF_PEST_flow.exe) to automatically run PEST to calibrate flow parameters associated with an HSPF simulation.

Checking to Ensure that PEST Files for Microbial Calibration are not Quarantined

Some personal computers contain Symantec security software that quarantines programs (usually executables, *.exe) when software is installed on the computer. We have experienced this issue with two files associated with the PEST installation:

- par2par.exe
- obsrep.exe

The user needs to confirm that these two files have not been quarantined. This can be done by confirming that the files are in the PEST folder:

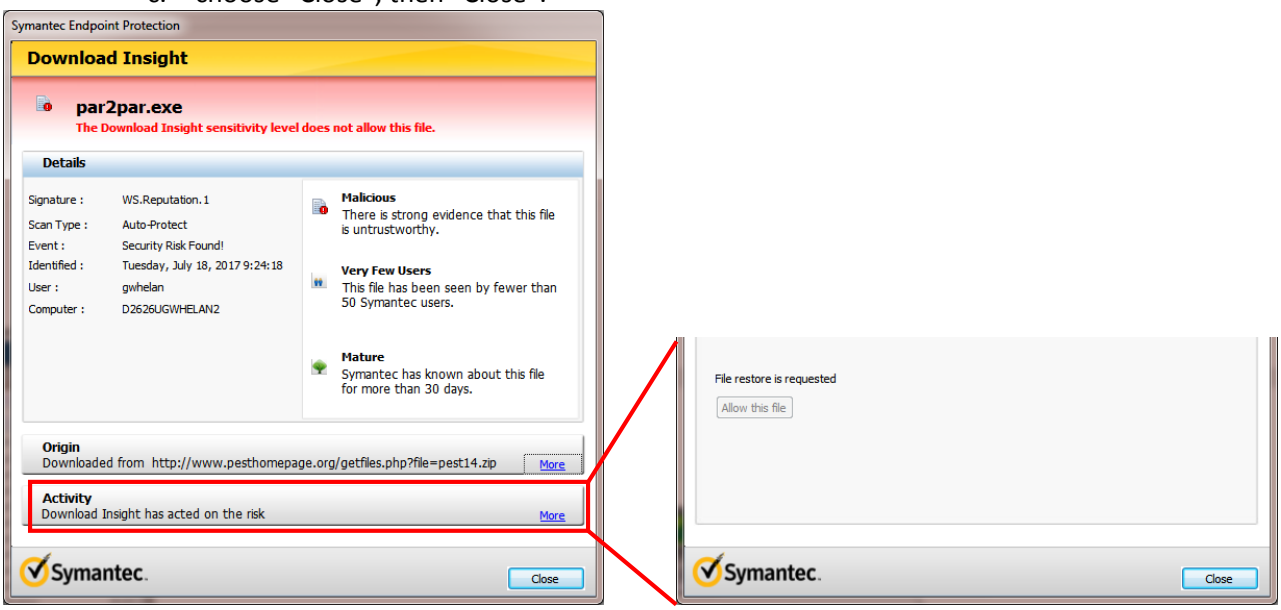


If the files do not appear in the folder, then the user needs to restore these files to the folder. This can be done a number of ways:

- The Symantec system will notify the user that a file has been quarantined.
- The Symantec icon can be used to change the settings

Symantec Notifies the User

3. If the user is notified, a screen similar to the following will appear. To change the setting,
    a. click “More” under “Activity”
    b. choose to “Allow this file”
    c. choose “Close”, then “Close”.

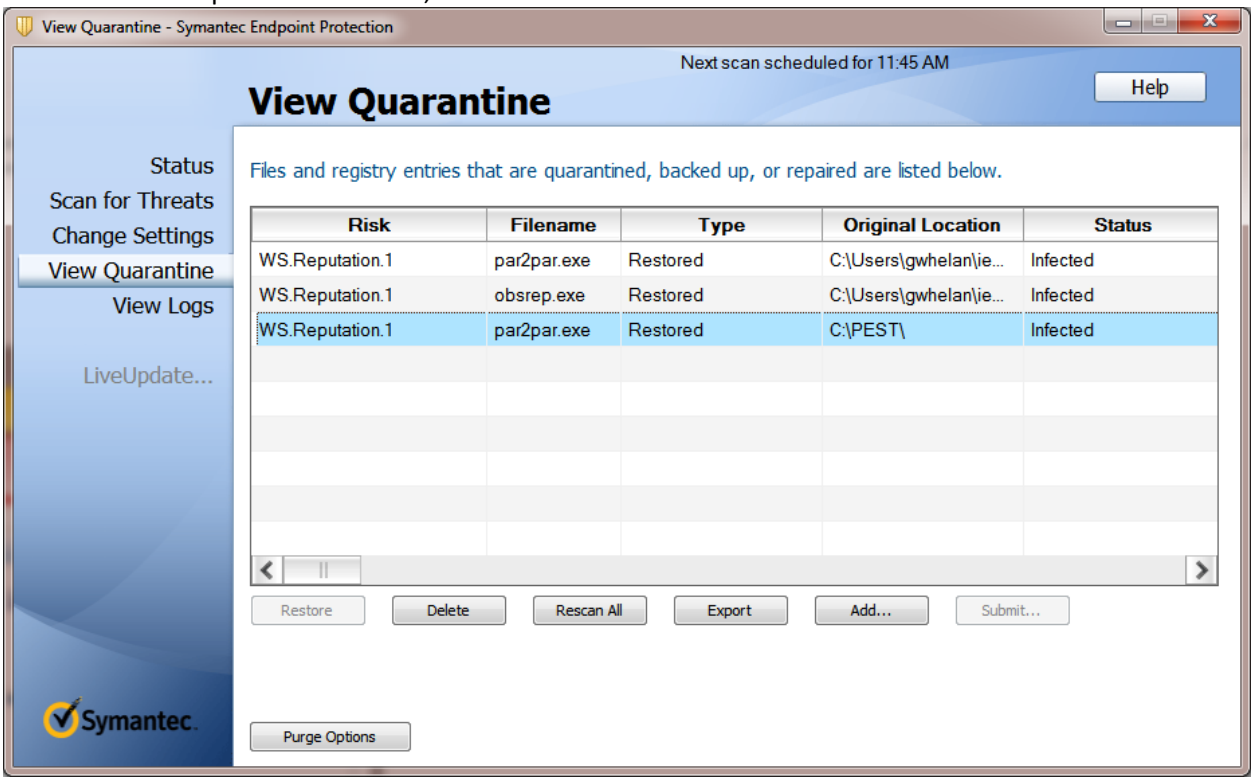


User Accesses the Symantec Icon

4. If the user is not notified about files being quarantined, then access the Symantec icon and change the settings:
    a. Go to the icon listing, usually on the bottom right of the user's home screen
    b. Choose the Symantec icon.

5. To restore quarantined files,
    a. choose "View Quarantine",
    b. right click on each file name,
    c. choose "Restore" from the list.

    Under "Type", "Quarantined" will be changed to "Restored", as illustrated in the following screen capture. Exit the file, and check to ensure the files have been restored to the PEST folder.



DISCLAIMER

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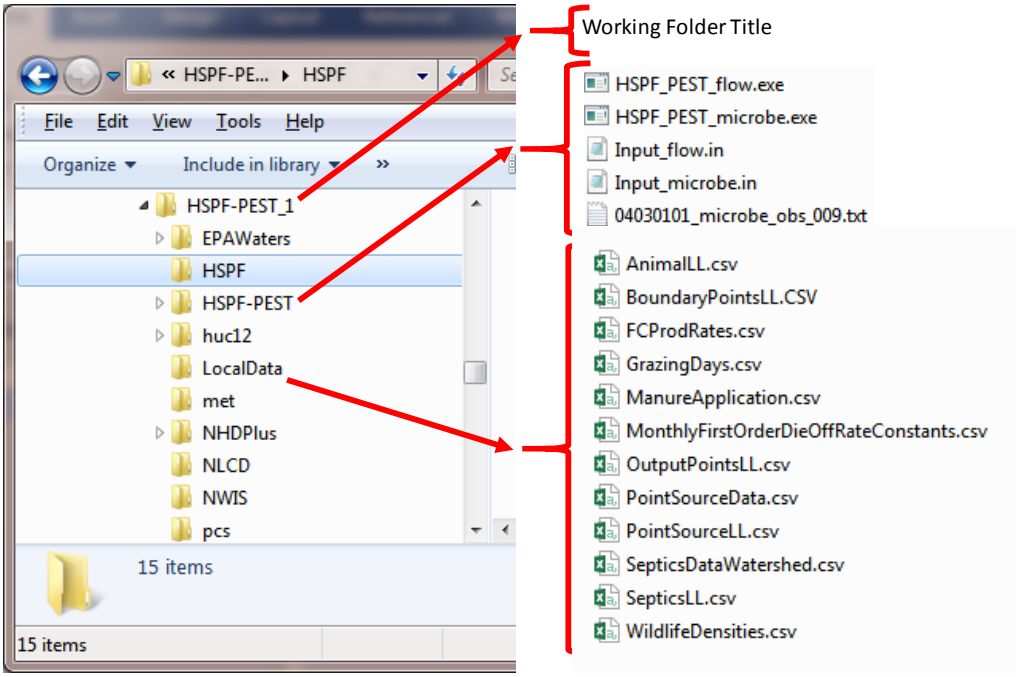
APPENDIX A
Example Folder Structure when Implementing a Site Assessment using the SDMProjectPuilder

When the SDMProjectBuilder is executed (i.e., SDMProjectBuilder.exe) on a specific site (e.g., see Whelan et al., 2017XX), the following files are automatically transferred from the user-defined SDMPB installation folder to user-defined site-specific working subfolders (HSPF-PEST and LocalData):

- **HSPF-PEST** – HSPF and PEST related calibration files for flow and microbes
  - Input_flow.in, which is an example input file containing the flow parameters used in the HSPF calibration process, as well as default input files that contain folder locations of HspfLt [batch (or light) version of HSPF], observed data used in the calibration, and PEST
  - HSPF_PEST_flow.exe, executable compiled with FORTRAN that prepares the inverse model PEST input files for HSPF flow parameter calibrations
  - Input_microbe.in, which is an example input file containing the microbial parameters used in the HSPF calibration process, as well as default input files that contain folder locations of HspfLt [batch (or light) version of HSPF], observed data used in the calibration, and PEST
  - HSPF_PEST_microbe.exe, executable compiled with FORTRAN that prepares the inverse model PEST input files for HSPF microbial parameter calibrations
  - 04030101_microbe_obs_009.txt, which is a file that contains observed microbial densities (i.e., concentrations) at a sampling location [e.g., near the outfall (i.e., mouth)] of the watershed; these data are used in the microbial calibration tutorial.
- **LocalData –** Microbial Property Data and Source Files to Identify and Modify Contamination Sources and Input Parameters
  - 12 Local Data CSV files, which capture user-defined microbial properties, and microbial loading source terms and locations
  - "POTW Point Source Example.xlsx", which provides the POTW discharge time series for a Point Source example