**CACIE Tool #NN** – **STOMP Surface File to P2R Tool**

**ca-getmod\_srf.pl**

**Version** **1.0**

**QA**: **QA**

# Description and Purpose

The STOMP Surface File to P2R tool combines STOMP Surface File data for a selected solute from each P2R cell that intersects the model domain as listed in the model input file. Solute mass flux rates and cumulative values leaving the base of the model over the area of each P2R cell are written to a solute-specific text file. The tool must be executed once for each solute in the STOMP simulation.

# Functional Requirements

The following are the functional requirements (FR) of the STOMP Surface File to P2R tool:

FR-1: Read the file name for the STOMP input file, the name of the solute being processed, the units for the solute, the keyword “top” or “bot” to select STOMP Surface Files associated with the top or bottom of the model, and the model name as command line arguments. The “top” option will not be used for CA modeling since the STOMP Surface File outputs for model tops were not included in the STOMP input files.

FR-2: Read the STOMP input file to extract the STOMP Output Surface File names for the files associated with the P2R grid cells. This is done based on Surface Flux Card in the STOMP input file that specify STOMP Output Surface Files associated with the P2R grid cells.

FR-3: Read the STOMP Surface Files associated with the P2R grid cells, extracting solute mass flux rates and cumulative values for the solute identified in FR-1.

FR-4: Generate a comma delimited (CSV) file for the solute identified in FR-1 that includes solute mass flux rates and cumulative values for all P2R grid cells that intersect the model domain.

# Software Requirements Specifications

The Perl programming language was used to develop this script. The Perl v5.18.2 interpreter was used in conjunction with the “Scalar::Util” module.

# Software Design Description

Arguments:

The tool is executed from the command line in a Linux terminal in the following manner:

$ perl ca-getmod\_srfs.pl STOMP\_input\_file solute\_name solute\_units bot\_top model\_name

Where:

* “ca-getmod\_srf.pl” is the file name of the tool
* “STOMP\_input\_file” is the path/file name of the STOMP input file used to create the STOMP Surface Files
* “solute\_name” is the name of the solute being processed; must be one of the solutes listed in the “STOMP\_input\_file”
* “solute\_units” is the concentration units for the solute (e.g., “ci” or “kg” or “g”)
* “bot\_top” is a keyword (“top” or “bot”) that determines whether Surface Files for the top or bottom of the model will be processed
* “model\_name” is the name of the model being processed and is used as the prefix for the output files.

Input Files:

* STOMP input file – STOMP input file used to create the STOMP Surface Files
* STOMP Surface Files – Surface Files generated by Stomp for the P2R grid cells (as listed in the STOMP input file)

Output Files:

* P2R mass file ([model\_name]\_[solute\_name]\_[bot\_top].csv) – Solute mass flux rates and cumulative values leaving the base of the model over the area of each P2R cell
* P2R cumulative file ([model\_name]\_[solute\_name]\_cumulative\_[bot\_top].csv) – Solute cumulative values and times to 25%, 50%, 75% and 99% for each P2R cell in the model area (This file is used for checking purposes only)

Tool Runner:

The following is the shell script configuration that will be passed as an argument to the Tool Runner for qualified runs:

{directory path to repository}\tools\ ca-getmod\_srfs.pl “$INPUT1 $INPUT2 $INPUT 3 $INPUT4 $INPUT5”

The shell script variable (indicated by the “$”) will be set in the shell script with the path to the control file (refer to the section of this document describing “Input Files”).

* $INPUT1
  + Path and name of the STOMP input file to be used
* $INPUT2
  + Name of the solute being processed. This will also become part of the output name.
* $INPUT3
  + Units for the Output file (e.g. “ci” or “kg” or “g”)
* $INPUT4
  + Keyword (“bot” or “top”): models can generate surface files associated with the top of the model and/or the bottom of the model. This specifies which you wish to work with.
* $INPUT5
  + Name of the model. This will be part of the output name.

Code Review:

Sara Lindberg performed a code review on May 12, 2020. No impacts to other repository tools or library dependencies were identified for the STOMP Surface File to P2R tool.

# Requirements Traceability Matrix

The requirements traceability matrix for the STOMP Surface File to P2R tool is presented in Table 1.

| Table 1  Requirements Traceability Matrix | | |
| --- | --- | --- |
| **Functional Requirement ID** | **Acceptance Test ID** | **Test Case** |
| QA Level | CACIE- STOMP Surface File to P2R-IT-1 | Installation Test |
| FR-1, FR-4 | CACIE- STOMP Surface File to P2R-AT-1 | * Check that P2R mass output file name includes the correct model name, solute name, and bot\_top keyword (consistent with arguments). * Check that the solute name is listed in the comment lines at the beginning of the P2R mass output file is consistent with the solute\_name argument. * Check that the units listed in the header line of the P2R mass output file are consistent with the solute\_units argument. |
| FR-1, FR-2 | CACIE- STOMP Surface File to P2R-AT-1 | Check that all Surface Files for P2R cells listed in the STOMP input file ~Surface Flux Card are included in the P2R mass output file header line. These files can be identified by the file names “modflow\_ii-jj.srf” where ii is the P2R i-index and jj is the P2R j-index. |
| FR-3, FR-4 | CACIE- STOMP Surface File to P2R-AT-2 | Using Excel, compare mass flux rate and cumulative values for the target solute from two Surface Files to the respective values in the P2R mass output file with column header titles corresponding to the Surface File names (i.e., “modflow\_ii-jj” where ii is the P2R i-index and jj is the P2R j-index). Values should be identical from start time to end time.  Note: To find the correct solute in the STOMP surface file, review the surface file comments they list the order of the solutes in relation to the columns. |
| FR-3, FR-4 | CACIE- STOMP Surface File to P2R-AT-2 | Using Excel, sum all solute mass flux rate and cumulative value columns in the P2R mass output file resulting in totals for all P2R cells in the model area.  Compare these values (for all times, start to end) to the values in the corresponding Surface File that covers the entire model area (xxxx-mass-balance.srf, where xxxx is the name of the solute being processed). Differences should be less than 1E-3 percent. |

# Installation Test Plan and Acceptance Test Plan Cases

The installation test plan for STOMP Surface File to P2R is presented in Table 2 and the acceptance test plan cases for STOMP Surface File to P2R are presented in Table 3 through Table 6.

| Table 2  **STOMP Surface File to P2R Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **STOMP Surface File to P2R Installation Testing**  **CACIE-STOMP Surface File to P2R – IT-1** | | **Date:** | |
| **Tool Runner Log File Location for this test:** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **Testing Directory:** | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Tools Code Repository Directory: | | | |
| Navigate to the testing directory | | | |
| 1 | Invoke Tool runner and test the tool using ***runner\_run\_IT-1\_ STOMP Surface File to P2R.sh*** as follows: Open a Linux terminal and after navigating to the appropriate directory indicated  *./runner\_run\_IT-1\_STOMP Surface File to P2R.sh* | | |
| 2 | Verify Tool Runner and tool is invoked and executed. |  |  |

| Table 3  **STOMP Surface File to P2R Acceptance Test Plan Case 1** | | | | | |
| --- | --- | --- | --- | --- | --- |
| **STOMP Surface File to P2R Acceptance Testing**  **CACIE-STOMP Surface File to P2R – AT-1** | | | **Date:** | | |
| **Tool Runner Log File Location for this test:**  [**\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\v4-2\_getmod\_surf\AT-1**](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\v4-2_getmod_surf\AT-1) | | | **Test Performed By: [FIRST & LAST NAME]** | | |
| **Testing Directory:** [**\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\v4-2\_getmod\_surf\AT-1**](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\src2stomp) | | | | | |
| **Test Step** | **Test Instruction** | | **Expected Result** | | **Test Result  (Pass/Fail)** |
| Navigate to the Testing Directory | | | | | |
| 1 | Open a Linux terminal and after navigating to the appropriate directory indicated and execute the following command: ./***runner\_run\_at-1\_surface\_file\_to\_p2r.sh***. | | | | |
| 2 | Check that P2R mass output file name includes the correct model name, solute name, and bot\_top keyword | Model name, solute name and bot\_top keyword are consistent with arguments | |  | |
| 3 | Check that the solute name is listed in the comment lines at the beginning of the P2R mass output file | Solute name is consistent with the solute\_name argument | |  | |
| 4 | Check that the units listed in the header line of the P2R mass output file | Units are consistent with the solute\_units argument. | |  | |
| 5 | Check that all Surface Files for P2R cells listed in the STOMP input file ~Surface Flux Card are included in the P2R mass output file header line. | These files can be identified by the file names “modflow\_ii-jj.srf” where ii is the P2R i-index and jj is the P2R j-index. | |  | |
| Using Excel: | | | | | |
| 6 | Compare mass flux rate and cumulative values for the target solute from two Surface Files to the respective values in the P2R mass output file with column header titles corresponding to the Surface File names (i.e., “modflow\_ii-jj” where ii is the P2R i-index and jj is the P2R j-index). | | Values should be identical from start time to end time.  Note: To find the correct solute in the STOMP surface file, review the surface file comments they list the order of the solutes in relation to the columns. |  | |
| 7 | Sum all of the solute mass flux rate columns together to calculate a total solute mass flux rate value for all P2R cells in the model area.  Sum all the cumulative value columns together in the P2R mass output file to calculate a total cumulative value for all P2R cells in the model area. | | This results in 2 columns: one for total Mass Flux Rate and one for total Cumulative. | | |
| 8 | Compare the values from Step 2 (for all times, start to end) to the values in the corresponding Surface File that covers the entire model area (xxxx-mass-balance.srf, where xxxx is the name of the solute being processed). | | Differences should be less than 1E-3 percent |  | |

# Acceptance Test Report

To complete the Acceptance Testing use Appendix A. The two test cases are described as follows:

* Acceptance Test 1 is in Table A-1. It …
* Acceptance Test 2 is in Table A-2. It …

Details of these tests, when they were conducted, by whom, and if they Passed or Failed are in each table of Appendix A.

# User Guide

Execute the tool as follows:

perl ca-getmod\_srf.pl <STOMP\_input file> <solute\_name> <solute\_units> <bot\_top> <model\_name>

See section 4 for a description of all inputs.

# Tool Versions

This section details changes incorporated into each version of the **STOMP Surface File to P2R** tool.

* 1.0 – Tool was developed.

# Appendix A

**Completed Acceptance Test Cases**

# Appendix B

**Completed Installation Test**

| Table B-1  **STOMP Surface File to P2R Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **STOMP Surface File to P2R Installation Testing**  **CACIE-STOMP Surface File to P2R – IT-1** | | **Date:** | |
| **Tool Runner Log File Location for this test:** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **Testing Directory:** | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Tools Code Repository Directory: | | | |
| Navigate to the testing directory | | | |
| 1 | Invoke Tool runner and test the tool using ***runner\_run\_IT-1\_ STOMP Surface File to P2R.sh*** as follows: Open a Linux terminal and after navigating to the appropriate directory indicated  *./runner\_run\_IT-1\_STOMP Surface File to P2R.sh* | | |
| 2 | Verify Tool Runner and tool is invoked and executed. |  |  |