**CACIE Tool #14**– **Build Surface Flux Tool (ca\_build\_surface\_flux.py)**

**Version** **1.2**

**QA**: **QA**

# Description and Purpose

The Build Surface Flux tool reads a STOMP input file and extracts the grid card. The tool then reads a MODFLOW shapefile and extracts the corresponding grids that are within the STOMP grid coordinates. It then creates a ~surface flux card, mapping the STOMP grid into the MODFLOW grid.

# Functional Requirements

The following are the functional requirements (FR) of the Build Surface Flux tool:

FR-1: Parse arguments

FR-2: Extract STOMP Grid template (~Grid Card)

FR-3: Build x index values based on input file STOMP Grid template

FR-4: Build y index values based on input file STOMP Grid template

FR-5: Find all MODFLOW shapefile nodes that fall within the STOMP x-y boundaries (x1≤…<xn, y1≤…<yn)

FR-6: Find all applicable x-indices for each MODFLOW shapefile grid from FR-5

FR-7: Find all applicable y-indices for each MODFLOW shapefile grid from FR-5

FR-8: Write to surface flux card text file: for each MODFLOW grid from FR-5, summarize the relevant STOMP coordinate indices for each contaminant.

# Software Requirements Specifications

Programming Language and required modules/libraries:

* Python 3.6
* Libraries:
  + Pyshp
  + Shapefile
  + Datetime
  + Os
  + Argparse
  + Logging
  + itemgetter from operator

# Software Design Description

Arguments:

* -s: Name of Sim Model, default="Unknown"
* -i: the stomp input file containing the ~grid card
* -shp: shapefile that the stomp grid card is being mapped to
* -c: Constituents used in this model
* -v: Use this to bypass validation of the list of contaminate names
* -o: Directory and name of output file; default: output/{model}/{date}/\_solute\_flux\_card.txt
* -csv: location to create csv file to check shapefile grid to stomp grid conversion; default: csv/{model}/{date}/{model}\_grid\_conversion.csv
* -b: Turn on boundaries for solute flux and Aqueous Volumetric. example: BNS will turn on bottom, North, and South. example 2(default): B will turn on bottom only.

Input Files:

There are 2 required files:

* STOMP input file. This gives us the grid used by the stomp model
* ShapeFile. This file contains the grid the STOMP grid is going to mapped to

Output Files:

There are 3 files that are output.

* log/error\_modify\_cards\_log\_{date}.txt: file containing all log entries generated during execution
* csv/{model}/{date}/{model}\_grid\_conversion.csv (default): contains coordinates that were used in the mapping between the two grids
* output/{model}/{date}/\_solute\_flux\_card.txt (default): Contains the stomp ~Surface Flux Card that was generated.

Tool Runner:

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

* python directory path]/ca-surf/ca\_build\_surface\_flux.py -c {copc list} -shp {shape file} -i {stomp input} -s {ModelName} -o {output file}
* Basic usage: -c contaminates, -shp shape file to use, -i stomp input file to get grid card from, -s what model this is for, -o (optional) file name and directory to create the surface flux card

Code Review:

Code walkthrough was performed by Sara Lindberg on 06/11/2019. Subsequent updates to the code were reviewed by Sara Lindberg on 03/05/2020, 03/10/2020, and on 03/17/2020. The code relies on standard python libraries and consists of a single python file which references only the standard python libraries as noted in Section 3. No impacts to other repository tools or library dependencies were identified for the Build Surface Flux tool.

# Requirements Traceability Matrix

The requirements traceability matrix for the Build Surface Flux Tool is presented in Table 1.

| Table 1  Requirements Traceability Matrix | | |
| --- | --- | --- |
| **Functional Requirement ID** | **Acceptance Test ID** | **Test Case** |
| QA Level | IT-1 | Installation Test |
| FR-1 | ATC 1 step: 3.1 | Check log file “input data” values against arguments |
| FR-2 | ATC 1 step: 3.2 | Check the following in log file:   * “stomp grid size,” * stomp grid x,” “stomp grid y,” and * “stomp grid k” values   against STOMP input file “Grid Card” values |
| FR-3 | ATC 1 step: 3.3 | Check log file “stomp grid i” values against STOMP input file |
| FR-4 | ATC 1 step: 3.4 | Check log file “stomp grid j” values against STOMP input file |
| FR-5 | ATC 1 step: 3.5 | Check log file “shape\_file\_grids” values against STOMP x-y boundaries (x1≤…<xn, y1≤…<yn) |
| FR-6 | ATC 1 step: 3.6 | Check contaminants and x-indices for one node in rad[]\_surface\_flux.txt |
| FR-7 | ATC 1 step: 3.7 | Check contaminants and y-indices for one node rad[]\_surface\_flux.txt |
| FR-8 | ATC 1 step: 3.8 | Check rad[]\_surface\_flux.txt “grid” values against log file “node” values |

# Installation Test Plan and Acceptance Test Plan Cases

The installation test plan for Build Surface Flux Tool is presented in Table 2 and the acceptance test plan case for Build Surface Flux Tool is presented in Table 3.

| **Table 2**  **Build Surface Flux Tool Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **Build Surface Flux Tool Installation Testing**  **CACIE-Build Surface Flux Tool – IT-1** | | **Date:** | |
| **Tool Runner File Location for this test:**  **[PUT LINK TO THE DIRECTORY HERE]** | | **Test Performed By:** | |
| **Testing Directory: [PROVIDE LINK TO 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 installation as follows:  *./* *CACIE\_ca\_build\_surface\_flux\_IT-1.sh* | | |
| 2 | Verify Tool Runner is invoked and executed. | Tool runner log generated |  |
| 3 | Verify tool is invoked and executed. | ./log/error\_modify\_cards\_log\_YYYYMMDD.txt file generated with error message:  CRITICAL: Invalid inputs: ../ss/input\_SS  CRITICAL: File not found, exiting script. |  |

| Table 3 **Build Surface Flux Tool Acceptance Test Plan Case 1** | | | |
| --- | --- | --- | --- |
| **Build Surface Flux Tool Acceptance Testing**  **CACIE-Build Surface Flux Tool – AT-1** | | **Date:** | |
| **Tool Runner File Location for this test:**  **[PUT LINK TO THE DIRECTORY HERE]** | | **Test Performed By:** | |
| **Testing Directory: [PROVIDE LINK TO TESTING DIRECTORY]** | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Navigate to the Testing Directory | | | |
| 1 | Invoke Build Surface Flux tool by entering the following entering the following:  ./ca-surf\_rad1\_run\_ATC-1thru8.sh | |  |
| 2 | Print out the following files:   * [Testing\_Directory]\/ca-surf-test/log/error\_modify\_cards\_log\_yyyymmdd.txt * [Testing\_Directory]\/ca-surf-test \rad[]\_surface\_flux.txt * [Testing\_Directory]\/ca-surf-test\ ca-surf\_rad1\_run\_ATC-1thru8.sh   ([Testing\_Directory]\ca-surf-test\ss\input  … | |  |
| 3 | Compare generated output files (./ca-surf-test/log/error\_modify\_cards\_log\_yyyymmdd.txt and rad[]\_surface\_flux.txt) against ca-surf\_rad1\_run\_ATC-1thru8.sh and STOMP input file ([Testing\_Directory]\ca-surf-test\ss\input) as follows:  … | |  |
| 3.1 | Check the following values in log file:   * “stomp grid size,” * stomp grid x,” “stomp grid y,” and * “stomp grid k” values   against STOMP input file “Grid Card” values | Values are consistent |  |
| 3.2 | Check log file “stomp grid i” values against STOMP input file | Values are consistent |  |
| 3.3 | Check log file “stomp grid j” values against STOMP input file | Values are consistent |  |
| 3.5 | Check log file “shape\_file\_grids” values against STOMP x-y boundaries (x1≤…<xn, y1≤…<yn) | Values are consistent |  |
| 3.6 | Check contaminants and x-indices for one node in check rad[]\_surface\_flux.txt | Values are consistent |  |
| 3.7 | Check contaminants and y-indices for one node in check rad[]\_surface\_flux.txt | Values are consistent |  |
| 3.8 | Check rad[]\_surface\_flux.txt nodes against log file nodes | Values are consistent |  |
| 3.9 | Check rad[]\_surface\_flux.txt nodes against [model]\_grid\_conversion.csv as follows: | |  |
| 3.9.1 | Rad[]\_surface\_flux.txt: “2, srf/modflow\_xx-xx.srf,” | xx-xx. should match up with p2r I-J in the csv file |  |
| 3.9.2 | Rad[]\_surface\_flux.txt: “Solute Flux, , 1/yr, , Bottom, X, Xe, Y, Ye, 1, 1,” | Correspond to fields in csv:  x = i\_start  Xe = i\_end  Y = j\_start  Ye = j\_end |  |

# 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.

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

The Build Surface Flux tool will be invoked using the Tool Runner tool using a shell script as defined in Section 4. The following defines the arguments specific to the Build Surface Flux tool.

Command line Arguments:

-s: Name of Sim Model, defaults to “Unknown”

-i: location and name of the input file with the ~grid card to be used. Defaults to the sim template

-shp: shapefile with the ground water grid to be used

-c: Constituents used in this model

-o: Directory and name of output file; default: output/{model}/{date}/\_solute\_flux\_card.txt

-csv: location to create csv file to check shapefile grid to stomp grid conversion; default: csv/{model}/{date}/{model}\_grid\_conversion.csv

-b: turn on boundaries for solute flux and Aqueous Volumetric:

* example: BNS will turn on bottom, North, and South.
* example 2(default): B will turn on bottom only

# Tool Versions

This section details changes incorporated into each version of the **Build Surface Flux Tool**.

* 1.0 – Tool was developed.
  + Adding to the Tool Runner Approved Tool list and removed comments from output that were no longer needed.
* 1.1 – Corrected issue where could not read northing and easting values. Used to only allow whole numbers for easting/northing, now can be floats.
* 1.2 – Updated generated csv file to facilitate checking (no changes to functionality)

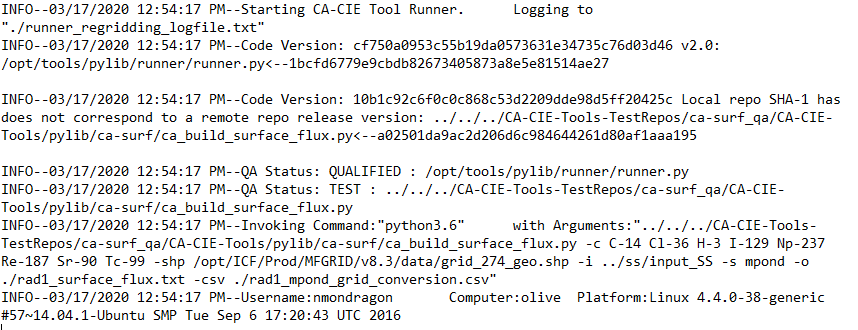
# Appendix A

**Completed Acceptance Test Cases**

**Testing Process Description**

The tool was executed using a shell file on linux, with the Tool Runner.

**Tool Runner Log**



| Table A-1 **Build Surface Flux Tool Acceptance Test Plan Case 1** | | | |
| --- | --- | --- | --- |
| **Build Surface Flux Tool Acceptance Testing**  **CACIE-Build Surface Flux Tool – AT-1** | | **Date: 3/17/2020** | |
| **Tool Runner File Location for this test: runner\_regridding\_logfile.txt** | | **Test Performed By: Neira Mondragon Oregon** | |
| **Testing Directory: Z:\CA-CIE-Tools-TestEnv\v4-2\_ca-surf\_test\ca-surf-QA-test** | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Navigate to the Testing Directory | | | |
| 1 | Invoke Build Surface Flux tool by entering the following entering the following:  ./ca-surf\_rad1\_run\_ATC-1thru8.sh | | Pass |
| 2 | Print out the following files:   * [Testing\_Directory]\/ca-surf-test/log/error\_modify\_cards\_log\_yyyymmdd.txt * [Testing\_Directory]\/ca-surf-test \rad[]\_surface\_flux.txt * [Testing\_Directory]\/ca-surf-test\ ca-surf\_rad1\_run\_ATC-1thru8.sh   ([Testing\_Directory]\ca-surf-test\ss\input  … | | Pass |
| 3 | Compare generated output files (./ca-surf-test/log/error\_modify\_cards\_log\_yyyymmdd.txt and rad[]\_surface\_flux.txt) against ca-surf\_rad1\_run\_ATC-1thru8.sh and STOMP input file ([Testing\_Directory]\ca-surf-test\ss\input) as follows:  … | | Pass |
| 3.1 | Check the following values in log file:   * “stomp grid size,” * stomp grid x,” “stomp grid y,” and * “stomp grid k” values   against STOMP input file “Grid Card” values | Values are consistent | Pass |
| 3.2 | Check log file “stomp grid i” values against STOMP input file | Values are consistent | Pass |
| 3.3 | Check log file “stomp grid j” values against STOMP input file | Values are consistent | Pass |
| 3.5 | Check log file “shape\_file\_grids” values against STOMP x-y boundaries (x1≤…<xn, y1≤…<yn) | Values are consistent | Pass |
| 3.6 | Check contaminants and x-indices for one node in check rad[]\_surface\_flux.txt | Values are consistent | Pass |
| 3.7 | Check contaminants and y-indices for one node in check rad[]\_surface\_flux.txt | Values are consistent | Pass |
| 3.8 | Check rad[]\_surface\_flux.txt nodes against log file nodes | Values are consistent | Pass |
| 3.9 | Check rad[]\_surface\_flux.txt nodes against [model]\_grid\_conversion.csv as follows: | | Pass |
| 3.9.1 | Rad[]\_surface\_flux.txt: “2, srf/modflow\_xx-xx.srf,” | xx-xx. should match up with p2r I-J in the csv file | Pass |
| 3.9.2 | Rad[]\_surface\_flux.txt: “Solute Flux, , 1/yr, , Bottom, X, Xe, Y, Ye, 1, 1,” | Correspond to fields in csv:  x = i\_start  Xe = i\_end  Y = j\_start  Ye = j\_end | Pass |

# Appendix B

**Completed Installation Test**

| **Table B-1**  **Build Surface Flux Tool Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **Build Surface Flux Tool Installation Testing**  **CACIE-Build Surface Flux Tool – IT-1** | | **Date:** | |
| **Tool Runner File Location for this test:**  **[PUT LINK TO THE DIRECTORY HERE]** | | **Test Performed By:** | |
| **Testing Directory: [PROVIDE LINK TO 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 installation as follows:  *./* *CACIE\_ca\_build\_surface\_flux\_IT-1.sh* | | |
| 2 | Verify Tool Runner is invoked and executed. | Tool runner log generated |  |
| 3 | Verify tool is invoked and executed. | ./log/error\_modify\_cards\_log\_YYYYMMDD.txt file generated with error message:  CRITICAL: Invalid inputs: ../ss/input\_SS  CRITICAL: File not found, exiting script. |  |

**Appendix C**

**QA Checklist**

