**CACIE Tool #15** – **Transient Output Card Generator Tool**

**OC\_rad\_gen.f**

**Version** **1.0**

**QA**: **QA**

# Description and Purpose

The Transient Output Card Generator tool creates the Output Control Card portion of a STOMP input file used for mass balance and transport production simulations. The Output Control Card details user selections for the contents of the STOMP-generated ***output*** file and one or more ***plot.xxx*** file(s), where ***xxx*** is the time step number for a simulation. The ***output*** file contains time-series of specified variable values at selected reference nodes. A ***plot.xxx*** file contains the variable values for all model nodes at a selected time. The tool is executed on Olive (Ubuntu  16.04.6 LT). Tool execution to create Output Control Cards should be limited to INTERA Vadose Zone modelers.

For both simulations, the Tool determines the reference nodes for a defined model domain. The reference nodes correspond to the center of the model domain and the center of each domain quadrant. If the model and/or quadrant centers are not located exactly at node centers, then the closest node center is chosen. The closest node center is determined by first evaluating i-index values, then j-index values. If a center location is equidistant (in i or j) from two node centers, then:

1) the lower i-index and j-index values are selected for the model center

2) the lower i-index value is selected for the western quadrants

3) the higher i-index value is selected for the eastern quadrants

4) the lower j-index value is selected for the southern quadrants

5) the higher j-index value is selected for the northern quadrants

The reference nodes are assigned vertically to the bottom of the domain, layer 20 and at successive layers at intervals of 20. The final layer interval corresponds to the elevation of the uppermost active layer at a reference node location (e.g., 1, 20, 40, …, 200, 208).

Reference node variables include:

* rock/soil type
* integrated water mass
* solute aqueous concentration (for each constituent modeled)
* solute integrated mass (for each constituent modeled)
* aqueous saturation
* aqueous moisture content
* aqueous pressure
* aqueous hydraulic head
* XNC aqueous volumetric flux (node centered)
* YNC aqueous volumetric flux (node centered)
* ZNC aqueous volumetric flux (node centered)

The reference nodes and reference node variables are identical in the Output Control Card files for both the mass balance simulation and the transport production simulation.

In the mass balance simulation Output Control Card file, a single plot time of 12,070 years is specified. In the transport production simulation Output Control Card file, plot times are defined in a file external to the Transient Output Card Generator tool (file name and location are provided as a command line argument).

Plot file output includes:

* rock/soil type
* solute aqueous concentration (for each constituent modeled)
* aqueous saturation
* aqueous moisture content
* aqueous pressure
* aqueous hydraulic head
* XNC aqueous volumetric flux (node centered)
* YNC aqueous volumetric flux (node centered)
* ZNC aqueous volumetric flux (node centered)
* no restart option

The plot time variables are identical in the Output Control Card files for both the mass balance simulation and the transport production simulation

# Functional Requirements

The following are the functional requirements of the Tool:

FR-1: Read radionuclide group (rad1 or rad2) and plot times file name and location as command line inputs.

* + rad1: C-14, Cl-36, H-3, I-129, Np-237, Re-187, Sr-90 and Tc-99
  + rad2: U‑232, U‑233, U‑234, U‑235, U‑236, U‑238, Th-230 and Ra-226

FR-2: Read input.sij from ../build. This file is generated using the CAST tool.

FR-3: Calculate model grid and quadrant center coordinates based on model area domain extent coordinates.

FR-4: Read ***input.nij*** from../build. This file is generated using the CAST tool.

FR-5: Determine model grid and quadrant center i/j- index values corresponding to the model grid and quadrant center coordinates (FR-3): i-index left/center/right and j-index bottom/center/top.

FR-6: Read ***input.top*** from ../build. This file is generated using the CAST tool.

FR-7: Determine top active layer for grid and quadrant centers.

FR-8: Read Output Card plot times (file name and location from command line input).

FR-9: Write Output Control Card for the transport production transport simulations (See Section 1 Description and Purpose for specifics).

FR-10: Write Output Control Card for the mass balance transport simulations (See Section 1 Description and Purpose for specifics).

# Software Requirements Specifications

FORTRAN, linux Intel(R) Fortran Intel(R) 64 Compiler

Compiler Options: -o OutputFileName

Special Considerations: None

# Software Design Description

Flow:

The Tool performs the following steps:

1. Declare variables – Character and array variables are declared.
2. Read command line arguments – See the list defined below.
3. Assign input files.
4. Open the output files.
5. Read model node boundary coordinates – Read model node edge x and y values from ***input.sij***.
6. Calculate grid and quadrant center locations based on coordinates read in Step 5.
7. Read model node center coordinates – Read model node center x and y values from ***input.nij***.
8. Calculate grid and quadrant center i/j index values corresponding to the grid and quadrant center coordinates from Step 6 using rules defined in Section 1 Description and Purpose.
9. Read tops – Read the uppermost active model layer for each i,j column in the model from ***input.top***.
10. Find top active layer for grid and quadrant centers from Step 8.
11. Calculate number of output layers for grid and quadrant centers.
12. Read Output Card plot times.
13. Write Output Control Card for the transport production transport simulations.
14. Write Output Control Card for the mass balance transport simulations.

Arguments:

RadGroup – Radionuclide group selected – rad1 or rad2.

* Radionuclide group 1 includes: C-14, Cl-36, H-3, I-129, Np-237, Re-187, Sr-90 and Tc-99.
* Radionuclide group 2 includes: U 232, U 233, U 234, U 235, U 236, U 238, Th-230 and Ra-226.

PlotTimes – Name and location of the file that contains the plot times to be used.

Input Files:

***input.sij*** (from ../build)

***input.nij*** (from ../build)

**input.top** (from ../build)

PlotTimes (name and location from command line argument; current location is in the ICF: /opt/ICF/Prod/TRPLYR/)

Output Files:

***rad#\_Output\_Control.dat***, where # is RadGroup (1 or 2) – Output Control Card file for production simulations.

***rad#\_ Mass\_Balance\_Output\_Control.dat***, where # is RadGroup (1 or 2) – Output Control Card file for mass balance simulations.

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-radocard/linux/OC\_rad\_gen\_linux-intel-64.exe {RadGroup} {PlotTimes}

Code Review:

A code review was performed by Sara Lindberg on 3/13/2020. No impacts to other repository tools or library dependencies were identified for the Transient Output Card Generator tool.

# Requirements Traceability Matrix

The requirements traceability matrix for the Transient Output Card Generator tool is presented in Table 1.

| Table 1  Requirements Traceability Matrix | | |
| --- | --- | --- |
| **Functional Requirement ID** | **Acceptance Test ID** | **Test Case** |
| QA Level | CACIE- OC\_rad\_gen-IT-1 | Installation Test |
| FR-1 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | Check that output files “*rad#\_Output\_Control.dat*” and “*rad#\_Mass\_Balance\_Output\_Control.dat*” (where # is 1 or 2, depending on radionuclide group read as command line input) were generated. |
| FR-1  FR-9  FR-10 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | Check that the radionuclide group input as a command line argument matches the radionuclide group in the output file names “*rad#\_Output\_Control.dat*” and *rad#\_ Mass\_Balance\_Output\_Control.dat*”, and that the radionuclides in the output files are correct for the selected the radionuclide group. |
| FR-2  FR-3  FR-4  FR-5 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | Check that reference nodes for model center and quadrant centers are at the center coordinates, or as close as possible, considering that model and quadrant centers may not fall exactly on a node center. |
| FR-6  FR-7 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | Check that the uppermost reference node at each i,j location is the top active node for that i,j location. |
| FR-8 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | Check that the plot times in *rad#\_Output\_Control.dat* (where # is 1 or 2, depending on radionuclide group read as command line input) agree with the times listed in the PlotTimes file (name and location from command line argument). |
| FR-9 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | For the production transport simulation Output Control Card file:  Check that the “Number of Reference Nodes” matches the number defined.  Check that the “Number of Reference Node Variables” matches the number defined.  Check that reference nodes are included for the model and quadrant centers for layer 1, the topmost active layer, and every layer number that is a multiple of 20 and less than the topmost active layer.  Check that the reference node variables are the expected parameters (See list in Section 1 Description and Purpose).  Check that number of plot times agrees with the number of times in the PlotTimes file (name and location from command line argument).  Check that the plot times match those in the PlotTimes file (name and location from command line argument).  Check that the “Number of Plot File Variables” matches the number defined.  Check that the plot file variables are the expected parameters (See list in Section 1 Description and Purpose). |
| FR-10 | CACIE-OC\_rad\_gen-TC-1  CACIE- OC\_rad\_gen-TC-2 | For the mass balance transport simulation Output Control Card file:  Check that the “Number of Reference Nodes” matches the number defined.  Check that the “Number of Reference Node Variables” matches the number defined.  Check that reference nodes are included for the model and quadrant centers for layer 1, the topmost active layer, and every layer number that is a multiple of 20 and less than the topmost active layer.  Check that the reference node variables are the expected parameters (See list in Section 1 Description and Purpose).  Check that there is a single plot file year at 12,070 years.  Check that the “Number of Plot File Variables” matches the number defined.  Check that the plot file variables are the expected parameters (See list in Section 1 Description and Purpose). |

# Installation Test Plan and Acceptance Test Plan Cases

The installation test plan for Transient Output Card Generator is presented in Table 2 and the acceptance test plan case for Transient Output Card Generator is presented in Table 3.

| Table 2  **Transient Output Card Generator Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **Transient Output Card Generator Installation Testing**  **CACIE-Transient Output Card Generator – IT-1** | | **Date:** | |
| **Tool Runner File Location for this test:**  **[PUT LINK TO THE DIRECTORY HERE]** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **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 installation of the tool as follows:  *./* *CACIE\_OC\_rad\_gen\_IT-1.sh* | | |
| 2 | Verify Tool Runner is invoked and executed. | Tool Runner log is generated and QA status documented |  |
| 3 | Verify tool is invoked and executed | rad1\_Mass\_Balance\_Output\_Control.dat and rad1\_Output\_Control.dat files are generated  Note: both files will be empty for installation test |  |

| Table 3 **Transient Output Card Generator Acceptance Test Plan Case 1** | | | |
| --- | --- | --- | --- |
| **Transient Output Card Generator Acceptance Testing**  **CACIE-Transient Output Card Generator – AT-1** | | **Date:** | |
| **Tool Runner File Location for this test:**  \\olive\backups\CAVE\v4-2Test\mpondOC\trOCcards\ | | **Test Performed By:** | |
| **Testing Directory:** \\olive\backups\CAVE\v4-2Test\mpondOC\ | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Qualified Input File Directory: S:\PSC\!HANFORD\ICF\Prod\TRPLYR\v1.0\data\plot\_times.txt | | | |
| 1 | Ensure the following files are in \\olive\backups\CAVE\v4-2Test\mpondOC\build, as they are needed for the execution of the ***OC\_rad\_gen.f*** tool:   * ***input.sij*** * ***input.nij*** * ***input.top*** | The expected files are present in the \\\olive\backups\CAVE\v4-2Test\mpondOC build directory. |  |
| 2 | Ensure that Navigate to the Qualified Input File Testing Directory contains the Plot Times file. | The Plot Times file is in the Qualified Input File Directory. |  |
| 3 | Execute, using a Linux terminal, the shell script ***runTR\_OC.sh*** in \trOCcards\ subdirectory of the testing directory. | The shell runs. |  |
| 4 | Confirm the following files were generated by ***OC\_rad\_gen.f*** in \trOCcards\ subdirectory of the testing directory:   * ***rad1\_Mass\_Balance\_Output\_Control.dat*** * ***rad1\_Output\_Control.dat*** * ***rad2\_Mass\_Balance\_Output\_Control.dat*** * ***rad2\_Output\_Control.dat***   Other files generated in the same directory that are not a functional requirement are as follows:   * ***rad1\_trOCcards\_Screen.log*** * ***rad2\_trOCcards\_Screen.log*** * ***tsurfcards\_.log*** | The files were generated in the testing directory. |  |
| 5 | Using a comparison program, such as DiffMerge, compare rad1\_Output\_Control.dat against rad2\_Output\_Control.dat. Confirm the only differences are: | | |
| 5.1 | * Line 3 – Depending on the file, either rad1 or rad2 will be on the line. | Either rad1 or rad2 is present on line 3 and is consistent with the respective filename prefix. |  |
| 5.2 | * Lines 108 to 123 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. |  |
| 5.3 | * Lines 193 to 200 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. |  |
| 6 | Using a comparison program, such as DiffMerge, compare rad1\_Mass\_Balance\_Output\_Control.dat against rad2\_Mass\_Balance\_Output\_Control.dat. Confirm the only differences are: | | |
| 6.1 | * Line 3 – Depending on the file, either rad1 or rad2 will be on the line. | Either rad1 or rad2 is present on line 3 and is consistent with the respective filename prefix. |  |
| 6.2 | * Lines 108 to 123 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. |  |
| 6.3 | * Lines 135 to 142 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. |  |
| 7 | Using a comparison program, such as “DiffMerge”, compare rad1\_Mass\_Balance\_Output\_Control.dat and rad1\_Output\_Control.dat. Confirm the following: | | |
| 7.1 | In the rad1\_Output\_Control.dat file:   * Line 131 should be the number of plot years that follow, which should be 59 * Lines 132 to 189 should match the listing in the Plot Times file. | The lines indicate the correct number of years and the correct years from the Plot Times file.  Line 131 value is the number of years listed in lines 132 to 189. |  |
| 7.2 | In the ***rad1\_Mass\_Balance\_Output\_Control.dat***:   * Line 131 should be the number of plot years that follow, which should be 1, * Line 132 should be 12070, year, | Line 131 value is 1,  Line 132 value is 12070, year, |  |
| If all the above passes then only one file from here to the end of the test will need to be checked, as all other items of the \*.dat files are the same.  Open the rad1\_Output\_Control.dat file for all proceeding test instructions. | | | |
| 8 | This Test Step will check the reference node profiles of the model domain. | | |
| 8.1 | Confirm the following sections are in the rad1\_Output\_Control.dat file:   * Center domain * Center first quadrant (upper right hand) * Center second quadrant (upper left hand) * Center third quadrant (lower left hand) * Center fourth quadrant (lower right hand) | These five domain/quadrants are present. |  |
| 8.2 | Confirm that the number of reference nodes on line 7 matches the number of reference node variable lines in the reference node profile section of the rad1\_Output\_Control.dat file.  The lines that follow have the following format: X, Y, Z, where X, Y, and Z are the I-, J-, and K- node index values, respectively, for the reference nodes. | The number of X, Y, and Z indices equals the value on line 7. |  |
| 8.3 | Navigate to the testing directory, the /build/ directory, and open input.sij.  The first line of this file contains two values: the number of X and Y nodes, respectively. Use these two values to calculate the I- and J- node values for the domain and quadrant centers in the rad1\_Output\_Control.dat file.  Confirm reference nodes of the model and quadrant centers correspond to the center coordinate, or as close as possible, according to the details described in Section 1.  Perform calculations in Excel and save the file in the testing directory, under /trOCcards/. | All five domain/quadrants are correctly calculated.  The Excel file containing the calculations is present in the described directory. |  |
| 8.4 | Open input.top in the /build/ directory of the testing directory.  In the rad1\_Output\_Control.dat file, the first set of node index values underneath each reference node profile heading for the model and quadrant centers represents the uppermost node in that domain/quadrant.  Using the uppermost node I- and J- values of each domain/quadrant verify the K-node index value matches the value in the third column of the input.top that corresponds to the same I- and J-node indices values of the uppermost node. | The first I-, J- and K- values of the Model and Quadrant Centers in rad1\_Output\_Control.dat match the values present within input.top. |  |
| 8.5 | Confirm in the rad1\_Output\_Control.dat file for each model and quadrant center reference node profile the K- representation starts at layer 1 (starts at the bottom row of each domain/quadrant), increments upward by 20 from layer 20 and the last layer is the topmost active layer.  For further details refer Section 1. | The Model and Quadrant Centers have correct K- value representation. |  |
| 9 | Confirm in the rad1\_Output\_Control.dat file the number on line 105 equals the number of lines that follow through the line ZNC Aqueous Volumetric Flux (Node Centers, mm/year,. | The number of plot variables match. |  |
| 10 | Aside from the radionuclides on lines 108 through 123 that were checked earlier in this Acceptance Test, confirm in the rad1\_Output\_Control.dat file the Reference Node Output Variables from lines 106 to 130 are the expected parameters described in Section 1. | The parameters match those listed in Section 1. |  |
| 11 | Confirm in the rad1\_Output\_Control.dat file the number of plot file variables on line 191 matches the number of lines to follow through the line No Restart, ,. | The number of plot variables match. |  |
| 12 | Aside from the radionuclides on lines 193 through 200 that were checked earlier in this Acceptance Test, confirm in the rad1\_Output\_Control.dat file the plot file variables from lines 192 through 207 are the expected parameters described in Section 1. | The parameters match those listed in Section 1. |  |
| 13 | Confirm in the rad1\_Output\_Control.dat file the second to last populated line in the rad1\_Output\_Control.dat indicates No Restart, , | Second to last line correctly states No Restart, , |  |

# Acceptance Test Report

To complete the Acceptance Testing use Appendix A. The single test case is the M Pond model for testing the ***OC\_rad\_gen.f*** tool, which generates four files:

* ***rad1\_Mass\_Balance\_Output\_Control.dat***
* ***rad1\_Output\_Control.dat***
* ***rad2\_Mass\_Balance\_Output\_Control.dat***
* ***rad2\_Output\_Control.dat***

Details of this test, when it was conducted, by whom, and if it Passed or Failed are in Table A-1 of Appendix A.

# User Guide

To run this code:

1. Copy the shell script runTR\_OC.sh from the /shell/ directory to the /ModelName/trOCcards/ subdirectory.
2. The /ModelName/build/ subdirectory must contain input.top, input.sij, and input.nij files.
3. Run the shell script in a Linux terminal using the runTR\_OC.sh command.
4. Ensure the four output files were created in the /ModelName/trOCcards/ subdirectory.

# Tool Versions

This section details changes incorporated into each version of the **Transient Output Card Generator** tool.

* 1.0 – Tool was developed.

# Appendix A

**Completed Acceptance Test Cases**

**Tool Runner Log – From the *tsurfcards\_.log* file**

INFO--03/12/2020 08:13:44 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:45 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py ../build/input.nij --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:45 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:45.121377

../build/input.nij d9fd84982198ea007f68c1ee2abcf9cf713fc94172a27f172f1fb1a3e7dd0d9d

INFO--03/12/2020 08:13:45 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:45 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py ../build/input.top --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:45 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:45.337299

../build/input.top e05cf2fad49da8c4a67fadb91d0d228b99085324111535028156e816a09bdde9

INFO--03/12/2020 08:13:45 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:45 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py /opt/ICF/Prod/TRPLYR/v1.0/data/plot\_times.txt --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:45 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:45.521036

/opt/ICF/Prod/TRPLYR/v1.0/data/plot\_times.txt c937409506327eebd17ff8963759698a23feab2f568b487c4753db35f426af2e

INFO--03/12/2020 08:13:45 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:45 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py ../build/input.sij --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:45 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:45.768416

../build/input.sij 7f123cab2d8401ca7fffd6ded637132e8fb180c6b768c305aa2e159c63cbfefb

INFO--03/12/2020 08:13:45 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:45 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:45 PM--Code Version: 3ae7e74b2198efed0dcbd87297efafce06b9997e Local repo SHA-1 has does not correspond to a remote repo release version: ../../../CA-CIE-Tools-TestRepos/repo\_OC\_rad\_gen.f/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe<--801301f995a74ad5b559a2681a401452aa7f4f5c

INFO--03/12/2020 08:13:45 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:45 PM--QA Status: TEST : ../../../CA-CIE-Tools-TestRepos/repo\_OC\_rad\_gen.f/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe

INFO--03/12/2020 08:13:45 PM--Invoking Command:"../../../CA-CIE-Tools-TestRepos/repo\_OC\_rad\_gen.f/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe" with Arguments:"rad1 /opt/ICF/Prod/TRPLYR/v1.0/data/plot\_times.txt"

INFO--03/12/2020 08:13:45 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

INFO--03/12/2020 08:13:46 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:46 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py rad1\_Output\_Control.dat --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:46 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:46.192691

rad1\_Output\_Control.dat 065478670c6f7a50e431719d8619f1ec76364c81c71abb67958ef7ed97bdb81a

INFO--03/12/2020 08:13:46 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:46 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py rad1\_Mass\_Balance\_Output\_Control.dat --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:46 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:46.444351

rad1\_Mass\_Balance\_Output\_Control.dat 964c965c4cb1f42fb8d79b51be68d1abf1238ce199bd2790e58df2e4ceda01e3

INFO--03/12/2020 08:13:46 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:46 PM--Code Version: 3ae7e74b2198efed0dcbd87297efafce06b9997e Local repo SHA-1 has does not correspond to a remote repo release version: ../../../CA-CIE-Tools-TestRepos/repo\_OC\_rad\_gen.f/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe<--801301f995a74ad5b559a2681a401452aa7f4f5c

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:46 PM--QA Status: TEST : ../../../CA-CIE-Tools-TestRepos/repo\_OC\_rad\_gen.f/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe

INFO--03/12/2020 08:13:46 PM--Invoking Command:"../../../CA-CIE-Tools-TestRepos/repo\_OC\_rad\_gen.f/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe" with Arguments:"rad2 /opt/ICF/Prod/TRPLYR/v1.0/data/plot\_times.txt"

INFO--03/12/2020 08:13:46 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

INFO--03/12/2020 08:13:46 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:46 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:46 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py rad2\_Output\_Control.dat --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:46 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:46.862015

rad2\_Output\_Control.dat f901709cab6e66e8d4cc3156a9c3d1ff5ec25b30f77c6e3f5f6245f3486b2b5a

INFO--03/12/2020 08:13:46 PM--Starting CA-CIE Tool Runner. Logging to "./trsurfcards\_.log"

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/12/2020 08:13:46 PM--Code Version: 147dee163e978f6038f4025817bca62529738e61 v1.16: /opt/tools/pylib/fingerprint/fingerprint.py<--13a885dc11cc15aea74c14b09c0d8584ec6cfd08

INFO--03/12/2020 08:13:47 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/12/2020 08:13:47 PM--QA Status: QUALIFIED : /opt/tools/pylib/fingerprint/fingerprint.py

INFO--03/12/2020 08:13:47 PM--Invoking Command:"python3.6" with Arguments:"/opt/tools/pylib/fingerprint/fingerprint.py rad2\_Mass\_Balance\_Output\_Control.dat --output ./trsurfcards\_.log --outputmode a"

INFO--03/12/2020 08:13:47 PM--Username:mweber Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

Fingerprint generated at 2020-03-12 20:13:47.090297

rad2\_Mass\_Balance\_Output\_Control.dat 1361b578a9364df935e47ccbeeeea2faa96be2faa13156f07c2fb53cc2d648e8

| Table A-1 **Transient Output Card Generator Acceptance Test Plan Case 1** | | | |
| --- | --- | --- | --- |
| **Transient Output Card Generator Acceptance Testing**  **CACIE-Transient Output Card Generator – AT-1** | | **Date: March 12, 2020** | |
| **Tool Runner File Location for this test:**  \\olive\backups\CAVE\v4-2Test\mpondOC\trOCcards\ | | **Test Performed By: M. Weber** | |
| **Testing Directory:** \\olive\backups\CAVE\v4-2Test\mpondOC\ | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Qualified Input File Directory: S:\PSC\!HANFORD\ICF\Prod\TRPLYR\v1.0\data\plot\_times.txt | | | |
| 1 | Ensure the following files are in \\olive\backups\CAVE\v4-2Test\mpondOC\build, as they are needed for the execution of the ***OC\_rad\_gen.f*** tool:   * ***input.sij*** * ***input.nij*** * ***input.top*** | The expected files are present in the \\\olive\backups\CAVE\v4-2Test\mpondOC build directory. | PASS |
| 2 | Ensure that Navigate to the Qualified Input File Testing Directory contains the Plot Times file. | The Plot Times file is in the Qualified Input File Directory. | PASS |
| 3 | Execute, using a Linux terminal, the shell script ***runTR\_OC.sh*** in \trOCcards\ subdirectory of the testing directory. | The shell runs. | PASS |
| 4 | Confirm the following files were generated by ***OC\_rad\_gen.f*** in \trOCcards\ subdirectory of the testing directory:   * ***rad1\_Mass\_Balance\_Output\_Control.dat*** * ***rad1\_Output\_Control.dat*** * ***rad2\_Mass\_Balance\_Output\_Control.dat*** * ***rad2\_Output\_Control.dat***   Other files generated in the same directory that are not a functional requirement are as follows:   * ***rad1\_trOCcards\_Screen.log*** * ***rad2\_trOCcards\_Screen.log*** * ***tsurfcards\_.log*** | The files were generated in the testing directory. | PASS |
| 5 | Using a comparison program, such as DiffMerge, compare rad1\_Output\_Control.dat against rad2\_Output\_Control.dat. Confirm the only differences are: | | |
| 5.1 | * Line 3 – Depending on the file, either rad1 or rad2 will be on the line. | Either rad1 or rad2 is present on line 3 and is consistent with the respective filename prefix. | PASS |
| 5.2 | * Lines 108 to 123 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. | PASS |
| 5.3 | * Lines 193 to 200 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. | PASS |
| 6 | Using a comparison program, such as DiffMerge, compare rad1\_Mass\_Balance\_Output\_Control.dat against rad2\_Mass\_Balance\_Output\_Control.dat. Confirm the only differences are: | | |
| 6.1 | * Line 3 – Depending on the file, either rad1 or rad2 will be on the line. | Either rad1 or rad2 is present on line 3 and is consistent with the respective filename prefix. | PASS |
| 6.2 | * Lines 108 to 123 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. | PASS |
| 6.3 | * Lines 135 to 142 – The rad1 file will have the rad1 grouping list and the rad2 file will have the rad2 grouping list (see Section 2 for the list). | The radionuclide grouping list is consistent with the respective filename prefix and the list in Section 2 of this document. | PASS |
| 7 | Using a comparison program, such as “DiffMerge”, compare rad1\_Mass\_Balance\_Output\_Control.dat and rad1\_Output\_Control.dat. Confirm the following: | | |
| 7.1 | In the rad1\_Output\_Control.dat file:   * Line 131 should be the number of plot years that follow, which should be 59 * Lines 132 to 189 should match the listing in the Plot Times file. | The lines indicate the correct number of years and the correct years from the Plot Times file.  Line 131 value is the number of years listed in lines 132 to 189. | PASS  PASS |
| 7.2 | In the rad1\_Mass\_Balance\_Output\_Control.dat:   * Line 131 should be the number of plot years that follow, which should be 1, * Line 132 should be 12070, year, | Line 131 value is 1,  Line 132 value is 12070, year, | PASS  PASS |
| If all the above passes then only one file from here to the end of the test will need to be checked, as all other items of the \*.dat files are the same.  Open the rad1\_Output\_Control.dat file for all proceeding test instructions. | | | |
| 8 | This Test Step will check the reference node profiles of the model domain. | | |
| 8.1 | Confirm the following sections are in the rad1\_Output\_Control.dat file:   * Center domain * Center first quadrant (upper right hand) * Center second quadrant (upper left hand) * Center third quadrant (lower left hand) * Center fourth quadrant (lower right hand) | These five domain/quadrants are present. | PASS |
| 8.2 | Confirm that the number of reference nodes on line 7 matches the number of reference node variable lines in the reference node profile section of the rad1\_Output\_Control.dat file.  The lines that follow have the following format: X, Y, Z, where X, Y, and Z are the I-, J-, and K- node index values, respectively, for the reference nodes. | The number of X, Y, and Z indices equals the value on line 7. | PASS |
| 8.3 | Navigate to the testing directory, the /build/ directory, and open input.sij.  The first line of this file contains two values: the number of X and Y nodes, respectively. Use these two values to calculate the I- and J- node values for the domain and quadrant centers in the rad1\_Output\_Control.dat file.  Confirm reference nodes of the model and quadrant centers correspond to the center coordinate, or as close as possible, according to the details described in Section 1.  Perform calculations in Excel and save the file in the testing directory, under /trOCcards/. | All five domain/quadrants are correctly calculated.  The Excel file containing the calculations is present in the described directory. | PASS  File saved as test\_step\_8.3.xlsx |
| 8.4 | Open input.top in the /build/ directory of the testing directory.  In the rad1\_Output\_Control.dat file, the first set of node index values underneath each reference node profile heading for the model and quadrant centers represents the uppermost node in that domain/quadrant.  Using the uppermost node I- and J- values of each domain/quadrant verify the K-node index value matches the value in the third column of the input.top that corresponds to the same I- and J-node indices values of the uppermost node. | The first I-, J- and K- values of the Model and Quadrant Centers in rad1\_Output\_Control.dat match the values present within input.top. | PASS |
| 8.5 | Confirm in the rad1\_Output\_Control.dat file for each model and quadrant center reference node profile the K- representation starts at layer 1 (starts at the bottom row of each domain/quadrant), increments upward by 20 from layer 20 and the last layer is the topmost active layer.  For further details refer Section 1. | The Model and Quadrant Centers have correct K- value representation. | PASS |
| 9 | Confirm in the rad1\_Output\_Control.dat file the number on line 105 equals the number of lines that follow through the line ZNC Aqueous Volumetric Flux (Node Centers, mm/year,. | The number of plot variables match. | PASS |
| 10 | Aside from the radionuclides on lines 108 through 123 that were checked earlier in this Acceptance Test, confirm in the rad1\_Output\_Control.dat file the Reference Node Output Variables from lines 106 to 130 are the expected parameters described in Section 1. | The parameters match those listed in Section 1. | PASS |
| 11 | Confirm in the rad1\_Output\_Control.dat file the number of plot file variables on line 191 matches the number of lines to follow through the line No Restart, ,. | The number of plot variables match. | PASS |
| 12 | Aside from the radionuclides on lines 193 through 200 that were checked earlier in this Acceptance Test, confirm in the rad1\_Output\_Control.dat file the plot file variables from lines 192 through 207 are the expected parameters described in Section 1. | The parameters match those listed in Section 1. | PASS |
| 13 | Confirm in the rad1\_Output\_Control.dat file the second to last populated line in the rad1\_Output\_Control.dat indicates No Restart, , | Second to last line correctly states No Restart, , | PASS |

# Appendix B

**Completed Installation Test**

**Tool Runner Log –**

INFO--03/19/2020 12:57:26 PM--Starting CA-CIE Tool Runner. Logging to "./trOCcards\_install\_test.log"

INFO--03/19/2020 12:57:26 PM--Code Version: 19633fecf43ac8ef2c4424bfe19fd563fc966f1b v2.1: /opt/tools/pylib/runner/runner.py<--1bcfd6779e9cbdb82673405873a8e5e81514ae27

INFO--03/19/2020 12:57:26 PM--Code Version: cf750a0953c55b19da0573631e34735c76d03d46 v2.0: ../../../CA-CIE-Tools-TestRepos/install\_repo/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe<--801301f995a74ad5b559a2681a401452aa7f4f5c

INFO--03/19/2020 12:57:26 PM--QA Status: QUALIFIED : /opt/tools/pylib/runner/runner.py

INFO--03/19/2020 12:57:26 PM--QA Status: QUALIFIED : ../../../CA-CIE-Tools-TestRepos/install\_repo/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe

INFO--03/19/2020 12:57:26 PM--Invoking Command:"../../../CA-CIE-Tools-TestRepos/install\_repo/tools/ca-radoccard/linux/OC\_rad\_gen\_linux-intel-64.exe" with Arguments:"rad1 infile3"

INFO--03/19/2020 12:57:26 PM--Username:slindberg Computer:olive Platform:Linux 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016

| Table B-1  **Transient Output Card Generator Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **Transient Output Card Generator Installation Testing**  **CACIE-Transient Output Card Generator – IT-1** | | **Date: 03/19/2020** | |
| **Tool Runner File Location for this test:**  **O:\CAVE\CA-CIE-Tools-TestEnv\CA-CIE-Tools\_v2.X\_install\_tests\trOCcards** | | **Test Performed By: Sara Lindberg** | |
| **Testing Directory: O:\CAVE\CA-CIE-Tools-TestEnv\CA-CIE-Tools\_v2.X\_install\_tests\trOCcards** | | | |
| **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 installation of the tool as follows:  ./ CACIE\_OC\_rad\_gen\_IT-1.sh | | |
| 2 | Verify Tool Runner is invoked and executed. | Tool Runner log is generated and QA status documented | Pass |
| 3 | Verify tool is invoked and executed | rad1\_Mass\_Balance\_Output\_Control.dat and rad1\_Output\_Control.dat files are generated  Note: both files will be empty for installation test | Pass |

**Appendix C**

**QA Checklist**

