**CACIE Tool #NN** – **RTD IC Tool**

**ca-rtdic.pl**

**Version** **1.0**

**QA**: **QA**

# Description and Purpose

The RTD IC tool scans an input source card file and a steady-state STOMP input file and generates Initial Conditions Cards for RTD restarts. The tool reads a list of sites that will undergo removal, treatment, and disposal (RTD) and generates the STOMP Initial Conditions Card that zeros out solute concentrations down to the RTD depth over the source area.

# Functional Requirements

The following are the functional requirements (FR) of the RTD IC tool:

FR-1: Accept user input at the command line as arguments, including the STOMP source card, RTD Site list, steady-state STOMP input file, the output file name and path, and selected solute names to include in the initial condition card.

FR-2: Read the RTD sites and RTD depths (expressed as number of grid layers) from the RTD site list.

FR-3: Identify source sites in the source card file that are also in the RTD site list.

FR-4: For the identified RTD source sites (FR-3), read the Ktop max value (i.e., the maximum uppermost active node k value for any i/j column) from the grid card in the steady-state STOMP input file. The initial condition overwrite file will apply this Ktop max value as the maximum for all source zones and waste sites.

FR-5: For each RTD source site, determine new i/j/k indices for the initial condition overwrite. The imin, imax, jmin, jmax values will be unchanged from the STOMP source card. The Kmin value will be determined on a site-by-site basis using the following two steps: find the smallest Kmin for each RTD source site from the source card then subtract the RTD depth (expressed as number of grid layers) read in FR-3.

FR-6: For each unique source domain of each identified RTD source site, write an initial condition line for each solute (FR-1) that overwrites the initial solute concentrations with zero.

FR-7: Save output file (i.e. initial conditions card) to filename/path specified in argument read in FR-1.

# Software Requirements Specifications

The Perl programming language was used to develop this script. The Perl v5.18.2 interpreter was used. No other libraries or dependencies (except for script inputs) are included with, or in relation to, this script.

# Software Design Description

Arguments:

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

$ perl ca-rtdic.pl source\_card\_file RTD\_site\_file input\_SS output\_file solute\_list

Where:

* “ca-rtdic.pl” is the file name of the tool
* “source\_card\_file” is the path/file name of the .card file (output from the SRC2STOMP Tool) containing the source card information for the model
* “RTD\_site\_file” is the path/file name of the file listing all CA RTD sites including RTD depths (expressed both in feet and as the equivalent number of grid layers)
* “input\_SS” is the path/file name of the STOMP steady-state file which at a minimum must contain the Grid Card
* “output\_file” is the path/file name of the output file generated by this tool
* “solute\_list” is list of solutes assumed to be removed during RTD

Input Files:

Three input files are required:

* source\_card\_file – This file (output from the SRC2STOMP Tool) contains the STOMP Source Card information for the model. Refer to the documentation for the SRC2STOMP Tool for details.
* RTD\_site\_file – This file lists all CA RTD sites. It also includes the RTD depths (ft) and the RTD depths expressed as number of grid layers. Its structure is as follows:
  + The first 4 lines are comments (marked with the “#” sign)
  + Subsequent lines following represent waste site treatment depths on a site-by-site basis. The format is: “[Site\_Name], [depth\_in\_feet], [No. STOMP cells],”
* Steady-State STOMP Input File – This file is a full STOMP input file, of which the “Grid Card” is parsed out for use by the tool.

Output Files:

The output file is composed of some general comments at the beginning of the file, followed by a comment line identifying RTD site and STOMP Initial Condition Overwrite lines for each solute in the input “solute\_list” for the RTD site. The RTD site name comment line and STOMP Initial Condition Overwrite lines are included for each unique source domain of each RTD site in the model domain.

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-rtdic\ca-rtdic.pl “$INPUT1 $INPUT2 $INPUT3 $OUTPUT1 $RADS”

The shell script variable (indicated by the “$”) will be set in the shell script, also briefly described as follows:

* $INPUT1
  + Path and file name of STOMP source card file (generated by the SRC2STOMP tool)
* $INPUT2
  + Path and file name of the RTD sites. Refer to the “Input Files” subsection of the “Software Design Description” section in this document for its format description
* $INPUT3
  + Path and file name of the STOMP steady-state input file
* $OUTPUT1
  + Path and file name of the desired output file
* $RADS
  + A list of analytes that will be written to the output file. In practice, the analytes included in this list will be the analytes removed from the cells described by $INPUT1 and $INPUT2.

Code Review:

Jacob Fullerton performed a code review on May 4th, 2020. No impacts to other repository tools or library dependencies were identified for the RTD IC tool.

# Requirements Traceability Matrix

The requirements traceability matrix for the RTD IC tool is presented in Table 1.

| Table  Requirements Traceability Matrix | | |
| --- | --- | --- |
| **Functional Requirement ID** | **Acceptance Test ID** | **Test Case** |
| QA Level | CACIE- RTD IC-IT-1 | Installation Test |
| FR-1 | CACIE- RTD IC-AT-1 | Execute the tool with user-specified inputs. Verify that the tool executes without errors and the proper outputs are generated with the specified solutes in the output file. |
| FR-2, FR-3 | CACIE- RTD IC-AT-1 | Compare the sites listed in the source card file to those listed in the RTD site file. Check that all sites that are found in both the source card file and the RTD site file are included in the output file Overwrite statements. |
| FR-4 | CACIE- RTD IC-AT-1 | The Ktop max values in the Overwrite statements should match the steady-state STOMP input card Ktop max value. |
| FR-5 | CACIE-RTD IC-AT-1 | The Kmin values should be constant per each site (regardless of variations in source card) for each overwrite statement, and should match up on a site-by-site basis with the corresponding Kmin value of each site. The imin, imax, jmin, and jmax values should match between the source card and Overwrite statements. |
| FR-6 | CACIE- RTD IC-AT-1 | Check that there is an Overwrite for each solute listed in the solute\_list (read from the command line arguments) for each unique source domain (i.e., same imin, imax, jmin, jmax, kmin, kmax) for each RTD site. |
| FR-7 | CACIE- RTD IC-AT-1 | Output file generated with the output file name/path specified in FR-1. |

# Installation Test Plan and Acceptance Test Plan Cases

The installation test plan for RTD IC is presented in Table 2 and the acceptance test plan case for RTD IC is presented in Table 3.

| Table  **RTD IC Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **RTD IC Installation Testing**  **CACIE-RTD IC – IT-1** | | **Date:** | |
| **Tool Runner Log File Location for this test:** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **Testing Directory:** [**\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd\_ic**](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd_ic) | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Tools Code Repository Directory: [\\olive\backups\CAVE\CA-CIE-Tools-TestRepos](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestRepos) | | | |
| Navigate to the testing directory | | | |
| 1 | Invoke Tool runner and test the tool using ***runner\_run\_IT-1\_RTD-IC.sh*** as follows: Open a Linux terminal and after navigating to the appropriate directory indicated type  *./runner\_run\_IT-1\_RTD-IC.sh* | | |
| 2 | A new directory called “IT-1” should have been created. Navigate into ***./IT-1*** and open ***runlog\_IT-1\_RTD-IC.log***. In this file there should be the following line (first line of the file):  Can’t open ./IT-1/not\_a\_file file No such file or directory | If this error message is reported in the file indicated this satisfies the installation test. |  |

| Table  **RTD IC Acceptance Test Plan Case 1** | | | |
| --- | --- | --- | --- |
| **RTD IC Acceptance Testing**  **CACIE-RTD IC – AT-1** | | **Date:** | |
| **Tool Runner Log File Location for this test:** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **Testing Directory:** [**\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd\_ic**](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd_ic) | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Navigate to the Testing Directory | | | |
| 1 | Invoke Tool runner and execute the tool using ***runner\_run\_AT-1\_RTD-IC.sh***. Open a Linux terminal and after navigating to the appropriate directory indicated and execute the following command: *./runner\_run\_AT-1\_RTD-IC.sh* | | |
| 2 | A new directory should have been created: ***./AT-1*** | | |
| 3 | Open the ***./AT-1*** directory and verify that two new files called ***rads1-rtd-ic.txt*** and ***rtdic\_screen.log*** are in the folder (a third file is also produced, which is the Tool Runner log file).  In a text editor, open ***rtdic\_screen.log*** and verify that the file does not contain the phrase “Can’t open” or “No such file or directory”. Also verify that the word “error” (case-insensitive search) does not appear in the file. Finally, verify that lines 2 through 9 are written as follows:   * C-14 * Cl-36 * H-3 * I-129 * Np-237 * Re-187 * Sr-90 * Tc-99 | If the ***rads1-rtd-ic.txt*** is generated and the associated log file contains the text indicated without including the error messages specified, this satisfies the following FR:  FR-1 & FR-7 |  |
| 4 | Open ***./data\_files/ca-rtd-sites.txt*** and ***./data\_files/rads1-src.card***. Verify that the common sites between the two files consist of the following:   * SrcSite1 * SrcSite2 * SrcSite3   The way to verify this is to compare each site name listed after the key phrase “# Site = “ in ***rads1-src.card*** and compare this to the list in ***ca-rtd-sites.txt***.  Open ***./AT-1/rads1-rtd-ic.txt*** and verify that the only sites in the file are the three sites listed above. The sites in ***rads1-rtd-ic.txt*** will be listed after the same key phrase used in ***rads1-src.card*** (“# Site = “, within quotes) | If only the three sites are present in the Overwrite file, this satisfies the following FR’s:  FR-2 & FR-3 |  |
| 5 | Open ***./data\_files/input\_SS*** and ***./AT-1/rads1-src.card***. In the ***input\_SS*** file, navigate to the “Grid Card” and find the Ktop value (the maximum number of nodes in the z-direction). The value should be 323. The way to read this is as follows, looking for the k-max value (highlighted):   * ~Grid Card * #----(optional comment line, commonly used) * Cartesian, * [i-max], [j-max], [k-max]   Open the ***rads1-rtd-ic.card*** file and verify that all of the Kmax values (the final number for each “Overwrite” line) are equal to 323. | If each Kmax value of the ***rads1-src.card*** matches the ***input­\_SS*** global Ktop value (323), this satisfies the following FR:  FR-4 |  |
| 6 | Open ***./AT-1/rads1-rtd-ic.txt*** and ***./data\_files/rads1-src.card*** in a text editor.  ###Part 1###  Verify that for each site the imin, imax, jmin, jmax values all match between the ***rads1-rtd-ic.txt*** and ***rads1-src.card*** files. The way these should “match” will be outlined for “SrcSite1”.  In ***rads1-src.card***, there are two different blocks of STOMP cells assigned sources, these different “blocks” within a waste site will be referred to as “zones” going forward. Each zone is written in STOMP notation using the following pattern: [i-min], [i-max], [j-min], [j-max], [k-min], [k-max]. In the ***rads1-src.card*** file, the two zones defined for “SrcSite1” are:   * 27, 30, 26, 28, 312, 312 * 31, 32, 26, 28, 310, 310   The imin, imax, jmin, and jmax values should be carried over verbatim from ***rads1-src.card*** to ***rads1-rtd-ic.txt*** for each analyte being overwritten. The analytes overwritten will be discussed/verified in a subsequent step.  Verify that the zones specified in ***rads1-src.card*** and ***rads1-rtd-ic.txt*** match for imin, imax, jmin, and jmax values for each source site.  ###Part 2###  Kmin should be uniform across all zones within each site in the ***rads1-rtd-ic.txt***. Kmin is obtained for each site by first finding the lowest Kmin for a site and then subtracting the appropriate depth as specified in the RTD site list. The following table will enumerate the expected findings.   |  |  |  |  | | --- | --- | --- | --- | | **Site** | **Local Kmin** | **RTD Depth (cells)** | **Final Kmin** | | SrcSite1 | 310 | 8 | 302 | | SrcSite2 | 311 | 13 | 298 | | SrcSite3 | 312 | 19 | 293 |   Verify that in ***rads1-rtd-ic.txt*** the corresponding Kmin for each site is used for each “Overwrite…” statement. | If the indices are written correctly to the ***rads1-rtd-ic.txt*** file as discussed in the instructions, this satisfies the following FR:  FR-5 |  |
| 7 | For each zone within each site of the ***./AT-1/rads1-rtd-ic.txt***, verify that there are “Overwrite” statements for each constituent specified. This means that SrcSite1, SrcSite2, and SrcSite3 all should have statements that start with “Overwrite Solute Volumetric Concentration,” immediately followed by the following constituents (one constituent per line):   * C-14 * Cl-36 * H-3 * I-129 * Np-237 * Re-187 * Sr-90 * Tc-99 | If all constituents are represented by each zone within each waste site, this satisfies the following FR:  FR-6 |  |

# Acceptance Test Report

To complete the Acceptance Testing use Appendix A. The test case is described as follows: Acceptance Test 1 is in Table A-1. This test executes the tool and validates the output against the input files.

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 <path/to/tool>ca-rtdic.pl <source\_card\_file/path> <RTD\_site\_file/path> <SS\_input\_file\_file/path> <output\_file/path> <solute\_list> <steady-state/STOMP/input/file>

# Tool Versions

This section details changes incorporated into each version of the **RTD IC** tool.

* 1.0 – Tool was developed.

# Appendix

**Completed Acceptance Test Cases**

**Tool Runner Log**

| Table A-1  **RTD IC Acceptance Test Plan Case 1** | | | |
| --- | --- | --- | --- |
| **RTD IC Acceptance Testing**  **CACIE-RTD IC – AT-1** | | **Date:** | |
| **Tool Runner Log File Location for this test:** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **Testing Directory:** [**\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd\_ic**](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd_ic) | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Navigate to the Testing Directory | | | |
| 1 | Invoke Tool runner and execute the tool using ***runner\_run\_AT-1\_RTD-IC.sh***. Open a Linux terminal and after navigating to the appropriate directory indicated and execute the following command: *./runner\_run\_AT-1\_RTD-IC.sh* | | |
| 2 | A new directory should have been created: ***./AT-1*** | | |
| 3 | Open the ***./AT-1*** directory and verify that two new files called ***rads1-rtd-ic.txt*** and ***rtdic\_screen.log*** are in the folder (a third file is also produced, which is the Tool Runner log file).  In a text editor, open ***rtdic\_screen.log*** and verify that the file does not contain the phrase “Can’t open” or “No such file or directory”. Also verify that the word “error” (case-insensitive search) does not appear in the file. Finally, verify that lines 2 through 9 are written as follows:   * C-14 * Cl-36 * H-3 * I-129 * Np-237 * Re-187 * Sr-90 * Tc-99 | If the log file contains the text indicated without including the error messages specified, this satisfies the following FR:  FR-1 | PASS |
| 4 | Open ***./data\_files/ca-rtd-sites.txt*** and ***./data\_files/rads1-src.card***. Verify that the common sites between the two files consist of the following:   * SrcSite1 * SrcSite2 * SrcSite3   The way to verify this is to compare each site name listed after the key phrase “# Site = “ in ***rads1-src.card*** and compare this to the list in ***ca-rtd-sites.txt***.  Open ***./AT-1/rads1-rtd-ic.txt*** and verify that the only sites in the file are the three sites listed above. The sites in ***rads1-rtd-ic.txt*** will be listed after the same key phrase used in ***rads1-src.card*** (“# Site = “, within quotes) | If only the three sites are present in the Overwrite file, this satisfies the following FR’s:  FR-2 & FR-3 | PASS |
| 5 | Open ***./data\_files/input\_SS*** and ***./AT-1/rads1-rtd-ic.txt***. In the ***input\_SS*** file, navigate to the “Grid Card” and find the Ktop value (the maximum number of nodes in the z-direction). The value should be 323. The way to read this is as follows, looking for the k-max value (highlighted):   * ~Grid Card * #----(optional comment line, commonly used) * Cartesian, * [i-max], [j-max], [k-max]   With the ***rads1-rtd-ic.txt*** file open in a text editor verify that all of the Kmax values (the final number for each “Overwrite” line) are equal to 323. | If each Kmax value of the ***rads1-rtd-ic.txt*** matches the ***input­\_SS*** global Ktop value (323), this satisfies the following FR:  FR-4 | PASS |
| 6 | Open ***./AT-1/rads1-rtd-ic.txt*** and ***./data\_files/rads1-src.card*** in a text editor.  ###Part 1###  Verify that for each site the imin, imax, jmin, jmax values all match between the ***rads1-rtd-ic.txt*** and ***rads1-src.card*** files. The way these should “match” will be outlined for “SrcSite1”.  In ***rads1-src.card***, there are two different blocks of STOMP cells assigned sources, these different “blocks” within a waste site will be referred to as “zones” going forward. Each zone is written in STOMP notation using the following pattern: [i-min], [i-max], [j-min], [j-max], [k-min], [k-max]. In the ***rads1-src.card*** file, the two zones defined for “SrcSite1” are:   * 27, 30, 26, 28, 312, 312 * 31, 32, 26, 28, 310, 310   The imin, imax, jmin, and jmax values should be carried over verbatim from ***rads1-src.card*** to ***rads1-rtd-ic.txt*** for each analyte being overwritten. The analytes overwritten will be discussed/verified in a subsequent step.  Verify that the zones specified in ***rads1-src.card*** and ***rads1-rtd-ic.txt*** match for imin, imax, jmin, and jmax values for each source site.  ###Part 2###  Kmin should be uniform across all zones within each site in the ***rads1-rtd-ic.txt***. Kmin is obtained for each site by first finding the lowest Kmin for a site and then subtracting the appropriate depth as specified in the RTD site list. The following table will enumerate the expected findings.   |  |  |  |  | | --- | --- | --- | --- | | **Site** | **Local Kmin** | **RTD Depth (cells)** | **Final Kmin** | | SrcSite1 | 310 | 8 | 302 | | SrcSite2 | 311 | 13 | 298 | | SrcSite3 | 312 | 19 | 293 |   Verify that in ***rads1-rtd-ic.txt*** the corresponding Kmin for each site is used for each “Overwrite…” statement. | If the indices are written correctly to the ***rads1-rtd-ic.txt*** file as discussed in the instructions, this satisfies the following FR:  FR-5 | PASS |
| 7 | For each zone within each site of the ***./AT-1/rads1-rtd-ic.txt***, verify that there are “Overwrite” statements for each constituent specified. This means that SrcSite1, SrcSite2, and SrcSite3 all should have statements that start with “Overwrite Solute Volumetric Concentration,” immediately followed by the following constituents (one constituent per line):   * C-14 * Cl-36 * H-3 * I-129 * Np-237 * Re-187 * Sr-90 * Tc-99 | If all constituents are represented by each zone within each waste site, this satisfies the following FR:  FR-6 | PASS |

# Appendix

**Completed Installation Test**

**Tool Runner Log**

| Table B-1  **RTD IC Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **RTD IC Installation Testing**  **CACIE-RTD IC – IT-1** | | **Date:** | |
| **Tool Runner Log File Location for this test:** | | **Test Performed By: [FIRST & LAST NAME]** | |
| **Testing Directory:** [**\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd\_ic**](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestEnv\rtd_ic) | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Tools Code Repository Directory: [\\olive\backups\CAVE\CA-CIE-Tools-TestRepos](file:///\\olive\backups\CAVE\CA-CIE-Tools-TestRepos) | | | |
| Navigate to the testing directory | | | |
| 1 | Invoke Tool runner and test the tool using ***runner\_run\_IT-1\_RTD-IC.sh*** as follows: Open a Linux terminal and after navigating to the appropriate directory indicated  *./runner\_run\_IT-1\_RTD-IC.sh* | | |
| 2 | A new directory called “IT-1” should have been created. Navigate into ***./IT-1*** and open ***runlog\_IT-1\_RTD-IC.log***. In this file there should be the following line (first line of the file):  Can’t open ./IT-1/not\_a\_file file No such file or directory | If this error message is reported in the file indicated this satisfies the installation test. |  |