**CACIE Tool #NN** – ***Composite Analysis STOMP Tool (ModelSetupFY18.jar)***

**Version** **1.0**

**QA**: **QA**

1. **Description and Purpose**

The Composite Analysis STOMP Tool (CAST) program is a graphical user interface (GUI) tool that produces STOMP input files based on user input model dimensions and material properties. A user will input the X, Y, and Z dimensions of a model and CAST will generate a comma-separated values (CSV) file containing each model grid center node within the user defined model boundary. That CSV will be used in a separate program, Kingdom2Stomp, and a second input to CAST will be the same CSV file with the addition of the geologic unit each model grid center node represents. Material properties can be mapped and visualized using CAST.

Only specific functions are utilized for the Composite Analysis (CA) 2020 project, so only the specific command windows identified in the steps that follow will be tested for QA. Specifically, the following Simulation Categories are not used nor put through this QA process:

* Simulation Controls
* Material Properties
* Zonation
* Geochemistry
* Initial Conditions
* Boundary Conditions
* Sources/Sinks
* Coupled Well Model
* Output Options

1. **Functional Requirements**

The following are the functional requirements of the CAST program:

FR-1: Ability to open and read a user provided configuration file that contains material and hydraulic properties.

FR-2: Input grid definition in CAST Grid option.

FR-3: Generate file containing top surface of the uppermost active node.

FR-4: Generate file containing the bottom surfaces of the bottom node.

FR-5: Generate STOMP input files.

1. **Software Requirements Specifications**

The programming language for the CAST tool is as follows:

Java, version 1.8.0\_231

1. **Software Design Description**

The following are required arguments for the CAST execution, necessary input files, and output files generated.

Arguments:

java -Dsun.java2d.dpiaware=false -jar -Djava.library.path={labrary path} -Xmx7000m -Xms7000m {name of \*.jar file}

* position 1: language argument leaves alone, unless gui is too big for screen in which case change to true
* Position 2: language argument leaves alone Position 3: This is the path of the application library. There should be a directory called “lib” in the same directory as ModelSetupFY18.jar
* Secondary Arguments (position 3 and 4): Allocate memory to be used
* Position 5: Directory path and filename of the *\*.jar* file for CAST execution

Input Files:

There are several files throughout the process of CAST use.

* The Configuration File, *\*-mdef.xml*
  + Basic model information is saved in this file
* An example file provided in examples/*200E-mdef.xml*
* An input file generated from Kingdom2Stomp, *ModelName-Eval.csv*, is used for mapping materials.

Output Files:

Two separate output file processes occur in the process of using CAST.

* The first output file generation is a single file with a X, Y, and Z columned CSV of all the model grid block node center locations, *ModelName.csv*. This file is generated from the LeapFrog program, and is used as an input for another tool, Kingdom2Stomp.
* The second output file generation produces 11 output files with the title *input*:
  + *input, input.bot, input.buildLog, input.east, input.nij, input.north, input.sij, input.south, input.top, input.west,* and *input.zone*
  + The *input.zone* file is a file with numbers for each model node representing the given geologic unit. Each line has 20 cells, each cell representing a specific model block. The file is constructed in that the first number represents the model block 1, 1, 1, the block in the southwest corner at the bottom of the model. Each successive number goes along the X-axis, from West to East until it reaches the end of the model grid row, and the moves to the next line along the Y-axis, 1, 2, 1. This pattern repeats until an entire Z-plane is complete, and then it moves up to the next Z-plane, 1, 1, 2. This process repeats for the entire model domain. Thus, the bottom of the *input.zone* file represents the top-most layer of the model. The last number in this file represents the northeastern corner of the top of the model.
  + The *input.bot* file is a four columned file representing each node of the model’s bottom layer and the grid cell surface, respectively. The value of -3 represents the bottom of the node.
  + The *input.nij* file represents the node count in the i-direction, node count in the j direction, X and Y for each model node center in plan view
  + The *input.sij* file represents the surface count in the i-direction, surface count in the j direction, X and Y for each model node corner in plan view.
  + The files *input.buildLog, input.north, input.south, input.west,* and *input.east* are not used in the Composite Analysis project, and therefore are not to be reviewed in this QA process.

Code Review:

There is no documentation linking the current version of the code to the executable that is currently in use. As we cannot verify the code belongs to the current executable, we will be deferring the code review until the next revision.

1. **Requirements Traceability Matrix**

The requirements traceability matrix for CAST are presented in Table 1.

| **Table 1 Requirements Traceability Matrix** | | |
| --- | --- | --- |
| **Functional Requirement ID** | **Acceptance Test ID** | **Test Case** |
| QA Level | CACIE-ModelSetupFY18.jar-IT-1 | Installation Test |
| FR-1 | CACIE- ModelSetupFY18.jar-TC-1 | Recognizing the model name |
| CACIE- ModelSetupFY18.jar-TC-2 | Test mapping the geologic materials |
| CACIE- ModelSetupFY18.jar-TC-3 | Activation of the configuration file in CAST |
| FR-2 | CACIE- ModelSetupFY18.jar-TC-1 | Test building model grid |
| CACIE- ModelSetupFY18.jar-TC-3 | Verification that the user-defined grid was translated into the input cards |
| FR-3 | CACIE- ModelSetupFY18.jar-TC-3 | Verify files generated by CAST |
| FR-4 |
| FR-5 | CACIE- ModelSetupFY18.jar-TC-3 | Verify files generated by CAST |

1. **Test Plan and Cases**

The Installation Test Plan for CAST is presented in Table 2 and the Acceptance Test Case Plan for CAST is presented in Table 3. Test Case 1, Building the Model Grid, steps through loading a template and adding X, Y, Z coordinates to it. Test Case 2, then builds on that to load material or geology from a csv file then map the correct materials/geology to the grid specified in the first test case. The Test Case 3 is the process to verify the first two cases completed and the outputs are accurate.

| **Table 2**  **CAST Installation Test Plan** | | | |
| --- | --- | --- | --- |
| **CAST Installation or Acceptance Testing**  **CACIE-** **ModelSetupFY18.jar-IT-1** | | **Date:** | |
| **Tool Runner File Location for this test:** | | **Test Performed By:** | |
| **Testing Directory:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST) Tool runs in Windows | | | |
| **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 cast using .bat file using below command:  *./runner\_run\_IT-1\_CAST.bat* | | |
| 2 | Verify Tool Runner is invoked and executed. | Tool runner file is generated.  Cast GUI interface is loaded. |  |
| 3 | Close the terminal window used to execute Tool Runner. | Window closes. |  |

| **Table 3**  **CAST Acceptance Test Plan** | | | |
| --- | --- | --- | --- |
| **CAST Acceptance Testing**  **CACIE-ModelSetupFY18.jar-AT-##** | | **Date:** | |
| **Tool Runner File Location for this test:** | | **Test Performed By:** | |
| **Testing Directory:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST\build](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST\build) Tool runs in Windows | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| **CACIE-** **ModelSetupFY18.jar-TC-1**  **Building the Model Grid** | | | |
| Navigate to the Testing Directory | | | |
| 1 | Invoke Tool runner and test the tool as follows:  *./runner\_run\_AT-1\_CAST.bat* | CAST GUI loads. |  |
| 2 | Click on /build/*acceptancetest1-mdef.xml* under Available Model Definition Files and click on the Revise button. | File is loaded. |  |
| 3 | In the Simulation Builder window revise the following fields:   * User Name: Insert your full first and last name * Organization/Company: Intera, Inc. * Title: Composite Analysis (CA) * Simulation Description:   + First line “QA Test Model”   + Second line should read “Steady-State Simulation,” | Details are correctly input in the Simulation Builder window. |  |
| 4 | Click on the Grid button under the Simulation Categories to open the Finite Difference Grid Builder window | Opens up the Finite Difference Grid Builder window. |  |
| 5 | In the STOMP Grid section be sure the following are selected:   * Grid Type: Cartesian * Elevation button * Specification: Manual | Values selected/input. |  |
| 6 | Under the X Surfaces section:   * Units: m * Definition Option: CSV * List Points: 567400,2@50,2@40,1@20,80@10,1@20,2@40,2@50, | Values selected/input. |  |
| 7 | Under the Y Surfaces section:   * Units: m * Definition Option: CSV * List Points: 135500,2@40,1@20,50@10,1@20,2@40, | Values selected/input. |  |
| 8 | Under the Z Surfaces section:   * Units: m * Definition Option: CSV * List Points: 126.9, [195@0.5](mailto:195@0.5) | Values selected/input. |  |
| 9 | Click Exit in the Finite Difference Builder window. | Window closes. |  |
| 10 | Click Save in the Numerical Model Setup window, type in your name, and click OK to save the changes. | *\*-mdef.xml* File is saved. |  |
| 11 | Click Material Mapping | Opens the Material Mapping window. |  |
| 12 | Click the Generate LeadFrog File button to open the window Generate LeapFrog File (XYZ CSV).  Input the file name as *test1.csv* and click OK. | Generates the *test1.csv* in the directory. |  |
| 13 | Click OK.  Click Exit.  Click Save in the Numerical Model Setup window, type in your name, and click OK to save the changes. | *\*-mdef.xml* File is saved. |  |
| 14 | In a separate program, such as Excel, create a file to calculate the node centers of each node within the model domain. Use the X, Y, and Z gridding from above.  This file will be titled and referred to as *calculated-nodes.\**, where the \* could be “xlsx” or any other user chosen file type. | A separated calculation file is created. |  |
| 15 | Compare the separate calculation file against the *test1.csv* file generated from CAST. | The two files match for each node center and the total number of nodes. |  |
| 16 | Proceed to CACIE-ModelSetupFY18.jar-TC-2 | | |
| **CACIE-** **ModelSetupFY18.jar-TC-2**  **Test Generating the Material Mappings** | | | |
| 1 | If you closed CAST after CACIE- ModelSetupFY18.jar-TC-1 then repeat steps 1 through 2 of CACIE- ModelSetupFY18.jar-TC-1. | The configuration file is loaded. |  |
| 2 | Click on Material Mapping | Opens the Material Mapping window. |  |
| 3 | In the Material Mapping section enter in the File Name: *test1-eval.csv* | File name is typed in. |  |
| 4 | Click Scan File for Codes at the base of the Material Mapping window | Read the eval file & populate the File Material Mapping section with two columns of data, Material Name and Code in File. |  |
| 5 | The Material Name cells will need to be selected based on the associated cell present in the Code in File column.   1. For Air the Material Name will be Inactive 2. For Surface Deposits the Material Name will be Backfill   For the rest of the units, the Material Name matches the Code in File. |  |  |
| 6 | Click the Preview button at the top of the Material Mapping window. | This will take a few moments to generate a separate window, Grid View, showing a three-dimensional representation of the grid and geology currently mapped. |  |
| 8 | Adjust the depth exaggeration to 10. | Subsurface is more visible |  |
| 9 | Confirm that the top of the model grid has at least a single grid cell of the top-most geologic unit (typically Backfill) present.  The geology looks appropriate for your model domain | User verifies at least one grid node present at uppermost layer. |  |
| 10 | Close the Grid View window. | Window closes. |  |
| 11 | Exit the Material Mapping window. | Window closes. |  |
| 12 | Click Save in the Numerical Model Setup window. | Saves. |  |
| 13 | Open Model Definition Selection window. | Window opens. |  |
| 14 | Select the model name you wish to create input files for, the *acceptancetest1-mdef.xml* in the File Name column under the Available Model Definition Files section. |  |  |
| 15 | Click the Generate Simulator Input File button at the bottom of the window. | Window opens. |  |
| 16 | Press OK with the default file name, input. | This will take several minutes.  The following output text will be generated in the command shell window when complete:  “Simulation Input File Build Completed Successfully at: [date/time]”. |  |
| 17 | In the build the folder the following files will be generated | input,  input.buildLog,  input.zone,  input.sij,  input.nij,  input.top,  input.bot,  input.north,  input.south,  input.west,  input.east |  |
| **CACIE-** **ModelSetupFY18.jar- TC-3**  **Verify Files Generated by CAST** | | | |
| 1 | Navigate to the Testing Directory, where the files from the final step of CACIE- ModelSetupFY18.jar-TC-2 were generated. | | |
| 1.1 | **Verify the *input.zone* file**  Node material numbers/values in the *input.zone* file should match material types in the Kingdom2Stomp output file, *test1-eval.csv*.  Use the calculation file created in step 14 of CACIE- ModelSetupFY18.jar-TC-1, *calculated-nodes.xlsx*, and *input.zone* for this Step. The *input.zone* file is described in Section 4. Software Design Description.  Create a copy of the *calculated-nodes.xlsx* file titled *zoned-calculated-nodes.xlsx*. Organize this file in the same way *input.zone* is:   * 20 nodes per line * The first cell in the file represents node center 1, 1, 1 * Last cell in the file represents the uppermost node in the northwestern top of the model * All other cells in between are in the same ordering as *input.zone* | The list of node centers is organized the same as *input.zone*. |  |
| 1.2 | Combine the material numbers in *input.zone* to the file *zoned-calculated-nodes.xlsx* in nearby columns, with blank columns in between. | Numbers added in file. |  |
| 1.3 | Add the material type to the file from the previous step based on the material list in the ~Rock/Soil Zonation Card in the *input* file. | Materials added in file. |  |
| 1.4 | Compare this file against the test1-eval.csv file. | Files match. |  |
| 2.1 | **Verify the *input.sij* file**  Use the *calculated-nodes.xlsx* file to calculate the southern grid edge of the model. | Southern edges are calculated. |  |
| 2.2 | Compare *input.sij* against *calculated-nodes.xlsx* to verify the files match | All nodes in the files match. |  |
| 3.1 | **Verify the *input.nij* file**  Use the *calculated-nodes.xlsx* file to calculate the northern grid edge of the model. | Northern edges are calculated. |  |
| 3.2 | Compare *input.nij* against *calculated-nodes.xlsx* to verify the files match | All nodes in the files match. |  |
| 4.1 | **Verify the *input.top* file**  Ensure the file contains the top surface of the uppermost active node in each ‘ij’ column.  Use the *calculated-nodes.xlsx* file to calculate the uppermost active node in each ij column. | Uppermost active nodes are calculated. |  |
| 4.2 | Compare *input.top* against *calculated-nodes.xlsx* to verify the files match. | All nodes in the files match. |  |
| 5.1 | **Verify the *input.bot* file**  Ensure the file contains the bottom surface plane nodes in each ij column.  Use the *calculated-nodes.xlsx* file to calculate the bottom layer of nodes in each ij column. | Bottom layer of nodes are calculated. |  |
| 5.2 | Compare *input.bot* against *calculated-nodes.xlsx* to verify the files match. | All nodes in the files match. |  |
| 6.0 | Open the *input* file and begin the verification process below. | | |
| 6.1 | **~Simulation Title Card**  Check that information in the ~Simulation Title Card matches entries in the Numerical Model Setup - Simulation Builder section of CAST | Matches. |  |
| 6.2 | **~Solution Control Card**  Check that information in the ~Solution Control Card matches entries on the CAST Simulation Controls page (selected from Numerical Model Setup page). | Matches. |  |
| 6.3 | **~Grid Card**  Check that information in the ~Grid Card matches entries on the CAST Grid page (selected from Numerical Model Setup page). | Matches. |  |
| 6.4 | **~Inactive Nodes Card**  Check that the *input.zone* zonation file is referenced. | Is referenced. |  |
| 6.5 | **~Rock/Soil Zonation Card**   * Check that the *input.zone* zonation file is referenced * Check that the material types listed in the *~Rock/Soil Zonation Card* match entries in the *Material Name* list (excluding Inactive) on the CAST Material Mapping page (selected from Numerical Model Setup page). | Is referenced & matches. |  |
| 6.6 | **~Mechanical Properties Card**  Check that information in the ~Mechanical Properties Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. |  |
| 6.7 | **~Hydraulic Properties Card**  Check that information in the ~Hydraulic Properties Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. |  |
| 6.8 | **~Saturation Function Card**  Check that information in the ~Saturation Function Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. |  |
| 6.9 | **~X-Aqueous Relative Permeability Card**  Check that information in the ~X-Aqueous Relative Permeability Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. |  |
| 6.10 | **~Y-Aqueous Relative Permeability Card**  Check that information in the ~Y-Aqueous Relative Permeability Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. |  |
| 6.11 | **~Z-Aqueous Relative Permeability Card**  Check that information in the ~Z-Aqueous Relative Permeability Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. |  |
| 6.12 | **~Initial Conditions Card**  Check that information in the ~Initial Conditions Card matches entries on the CAST Initial Conditions page (selected from Numerical Model Setup page). | Matches. |  |
| 6.13 | **~Boundary Conditions Card**  Check that information in the ~Boundary Conditions Card matches entries on the CAST Boundary Conditions page (selected from Numerical Model Setup page). Typically, for the steady-state models there are no boundary conditions. | Matches. |  |
| 6.14 | **~Source Card**  Check that information in the ~Source Card matches entries on the CAST Sources/Sinks page (selected from Numerical Model Setup page). typically, for the steady-state models there are no sources or sinks. | Matches. |  |
| 6.15 | **~Output Control Card**  Check that information in the ~Output Control Card matches entries on the CAST Output Specifications page (selected from Numerical Model Setup page). | Matches. |  |
| 6.16 | **~Surface Flux Card**  Check that information in the ~Surface Flux Card matches entries on the CAST Output Specifications page, Surface Flux tab (selected from Numerical Model Setup page). | Matches. |  |

1. **Acceptance Test Report**

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

* Acceptance Test 1 is in Table A-1. This has the user input X, Y, and Z gridding values for a model in 200W, LW Crib Area Model and generate the *ModelName.csv* file to be used as an input for the Kingdom2Stomp tool.
* Acceptance Test 2 is in Table A-2. This test maps the geologic materials in order to be used in Acceptance Test 3.
* Acceptance Test 3 is in Table A-3. This test generates the input files to be used in STOMP modeling and verifies the input files represent the user-specified model domain, appropriate gridding surfaces & planes, the associated geologic formations of each model node, and the pre-defined hydrologic and material properties.

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

1. **User Guide**

To start the application you will need to have Java installed. Once Java is installed you can execute the application with the below command in a command window:

Java -Dsun.java2d.dpiaware=false -jar -Djava.library.path=..\..\tools\tools\CAST\lib -Xmx7000m -Xms7000m ..\..\tools\tools\CAST\ModelSetupFY18.jar

For more information on arguments see section 4: Software Design Description. See Tool runner documentation for how to execute using ToolRunner application.

Model Grid Construction and Generating the Input Files

Building The Grid in CAST

* 1. Execute CAST
  2. Click on name of xml file under Available Model Definition Files and click on the Revise button.
  3. In the Simulation Builder window revise the following fields:
  4. User Name: Insert your full first and last name
     1. Organization/Company: Intera, Inc.
     2. Title: Composite Analysis (CA)
     3. Simulation Description: Insert the formal model name followed by “Model” For Example: A Farms Area Model. The second line should state the purpose of the model such as “Steady-State Simulation,”
  5. Click on the Grid button under the Simulation Categories to open up the Finite Difference Grid Builder window to revise the grid model surfaces (X, Y, and Z) specific to the model.
  6. In the STOMP Grid section be sure the following are selected:
     1. Grid Type: Cartesian
     2. Elevation radio button
     3. Specification: Manual
  7. Under the X Surfaces section the user will define the x-plane dimensions for the model. The Units will be meters (m) but the Definition Option is model domain-specific and will be selected by the modeler.
     1. For models with gridding that is of equal length in one direction across the domain, select Definition Option as Constant Grid Spacing and define the following:
        1. The Start node value, the Xmin value of the grid. Put a comma after this value.
        2. The DX value, which is equal to the length of each grid in the x-direction.
        3. The Nodes NX, which is the number of nodes of a DX value.
        4. The End value is calculated from the inputs provided
     2. For models with variable gridding across the domain, select Definition Option to be CSV and define the following in order in the List Points text box:
        1. The initial node value will be the Xmin value of the gird. Put a comma after this value.
        2. The next string of numbers and characters represent the number of nodes at a given meter distance along the x-axis, separated by an ‘@’ symbol. For example, if the user wants 35 nodes of 10 meter length they will put 35@10, It is important after each segment a comma is placed.
        3. Do not put a final node value. IE always end with a comma
        4. Example: 574600,35@10,60@5,25@10,
  8. Under the Y Surfaces section the user will define the y-plane dimensions for the model. The Units will be meters (m) but the Definition Option and List Points will be user specific.
     1. If the Definition Option is Constant Grid Spacing the user will define:
        1. The Start node value, the Ymin value of the grid. Put a comma after this value.
        2. The DY value, which is equal to the length of each grid in the y-direction.
        3. The Nodes NY, which is the number of nodes of a DY value.
        4. The End value is calculated from these inputs provided, which should match the Ymax value of the grid
     2. If the Definition Option is CSV the user will define, in order:
        1. The initial node value will be the Ymin valueof the grid. Put a comma after this value.
        2. The next string of numbers and characters represent the number of nodes at a given meter distance along the y-axis, separated by an ‘@’ symbol. For example, if the user wants 35 nodes of 10 meter length they will put 35@10, It is important after each segment a comma is placed.
        3. Do not put a final node value. IE always end with a comma
        4. Example: 134800,30@10,110@5,25@10,
  9. Under the Z Surfaces section the user will define the z-plane dimensions for the model. The Units will be meters (m) but the Definition Option and List Points will be user specific.
     1. If the Definition Option is Constant Grid Spacing the user will define:
        1. The Start node value, the Zmin value of the grid.
        2. The DZ value, which is equal to the length of each grid in the z-direction.
        3. The Nodes NZ, which is the number of nodes of a DZ value.
        4. The End value is calculated from these inputs.
     2. If the Definition Option is CSV the user will define in order:
        1. The initial node value will be the Zmin value fof the grid. Put a comma after this value.
        2. The next string of numbers and characters represent the number of nodes at a given meter distance along the z-axis, separated by an ‘@’ symbol. For example, if the user wants 150 nodes of 0.5 meter length they will put [150@0.5](mailto:150@0.5), It is important after each segment a comma is placed.
        3. Do not put a final node value.
        4. Example: [121.7,17@0.5,98@0.1,189@0.5](mailto:121.7,17@0.5,98@0.1,189@0.5),
  10. Check the Click Exit in the Finite Difference Builder window.
  11. Click Save in the Numerical Model Setup window, type in your name, and click OK to save the changes.
  12. Note, after recording revisions/saving CAST returns to the Model Definition Selection window. Click on the Revise button to continue with the next step.

## Material Mapping

* 1. From the Numerical Model Setup window click on the Material Mapping button under the Simulation Categories to open the Material Mapping window.
     1. Under the File Material Mapping section click on the Generate Leapfrog File button. A window, Generate LeapFrog File (XYZ CSV), appears asking the user to input a LeapFrog file name.
     2. For the file name enter the model name using no spaces followed by “.csv”. Example, afarms.csv
  2. Click OK.
     1. Note: Generation of this file takes several minutes—the CAST window interface does not include a progress indicator but the PowerWindow shell displays the following text: LeapFROG File Name = [ModelName].csv when script begins execution. Keep an eye on the windows explorer window to see the updated file size as it is built.
  3. A confirmatory dialog box will open when file generation is complete. Click OK to continue.
  4. Click Exit in the Material Mapping window.
  5. Click Save in the Numerical Model Setup window, type in your name, click OK to save the changes,

## Mapping the Geologic Units

* 1. Click on Material Mapping to open the Material Mapping window.
  2. In the File Material Mapping section enter in the CSV File Name section the name of your file (typically created by ArcGIS or Kingdom2stomp.
  3. Next click the button Scan File for Codes at the base of the Material Mapping window. This will read the eval file and populate the File Material Mapping section with two columns of data, Material Name and Code in File.
  4. The Material Name cells will need to be selected based on the associated cell present in the Code in File column.
     1. For Air the Material Name will be Inactive
     2. For Surface Deposits the Material Name will be Backfill
     3. For the rest of the units, the Material Name matches the Code in File
  5. Next, click the Preview button at the top of the Material Mapping window. This will take a few moments to generate a separate window, Grid View, showing a three-dimensional representation of the grid and geology currently mapped.
     1. Adjust the depth exaggeration to 10.
     2. Confirm the following:
        1. The top of the model grid has at least a single grid cell of the top-most geologic unit (typically Backfill) present
        2. The geology looks appropriate for your model domain
     3. Close the Grid View window,
  6. exit the Material Mapping window,
  7. click Save in the Numerical Model Setup window to record these revisions.

## Generating the Input Files

* 1. With the Model Definition Selection window open, select the model name you wish to create input files for, the ***xml*** file in the File Name column under the Available Model Definition Files section.
  2. Next click the Generate Simulator Input File button at the bottom of the window. This will open a new window asking the user to define the input file name. Press OK with the default file name, input.
     1. Note, this will take several minutes. The following output text will be generated in the command shell window when it is complete: “Simulation Input File Build Completed Successfully at: [date/time]”.
  3. In the build the folder the following files will be generated – ***input, input.buildLog, input.zone, input.sij, input.nij, input.top, input.bot, input.north, input.south, input.west, input.east.***

**Appendix A**

**Acceptance Testing Logs**

**Testing Process Description:**

All testing files are in olive/backups/CAVE/CA-CIE-Tools-TestEnv/v4-2\_CAST/build.

Test CACIE- ModelSetupFY18.jar-AT-1:

1. Renamed 200W-mdef.xml to acceptancetest1-mdef.xml.
2. Opened a DOS command window.
3. Performed CACIE- ModelSetupFY18.jar-AT-1 Test Steps 1 through 13 (as described in Table A-2 below).
4. Wrote the FORTRAN code calculated-nodes.f to list node XYZ values based on a grid definition file, grid\_def.txt, that contains grid info for the Test CACIE-ModelSetupFY18.jar-AT-1 model.
5. Executed code: ./calculated-nodes.exe > calculated-nodes.echo   
    ---> calculated-nodes.txt.
6. Compared calculated-nodes.txt (generated by calculated-nodes.exe) to test1.csv (generated from CAST)   
    in compare\_calculated-nodes.xlsx.
7. No differences: Test CACIE- ModelSetupFY18.jar-AT-1 passed.

Test CACIE-ModelSetupFY18.jar-AT-2:

1. Performed CACIE-ModelSetupFY18.jar-AT-2 Test Steps 1 through 17 (as described in Table A-3 below).
2. Test CACIE-ModelSetupFY18.jar-AT-2 passed.

Test CACIE-ModelSetupFY18.jar-AT-3:

1. Wrote the FORTRAN code input\_zone\_units.f to read the input and input.zone files and output a file listing i, j, k, x, y, z, material zone number and material name for each model node.
2. Executed code: ./input\_zone\_units.exe > input\_zone\_units.echo  
    ---> input\_zone\_materials.dat.
3. Compared input\_zone\_materials.dat (generated by input\_zone\_units.exe) to test1-eval.csv (provided in the test directory as input to CAST) in compare\_input\_zone.xlsx.
4. Units match: Test CACIE-ModelSetupFY18.jar-AT-3, Test Steps 1.1 to 1.4 (as described in Table A-4 below) passed.
5. Compared input.sij (output from CAST) to calculated values in compare\_input\_sij.xlsx.
6. Values match: Test CACIE-ModelSetupFY18.jar-AT-3, Test Steps 2.1 to 2.2(as described in Table A-4 below) passed.
7. Compared input.nij (output from CAST) to calculated values in compare\_input\_nij.xlsx.
8. Values match: Test CACIE-ModelSetupFY18.jar-AT-3, Test Steps 3.1 to 3.2(as described in Table A-4 below) passed.
9. Imported input\_zone\_materials.dat (generated by input\_zone\_units.exe) toExcel and calculated uppermost active node in each ij column ---> compare\_input\_top.xlsx.
10. Compared calculated top values to input.top (output from CAST) in compare\_input\_top.xlsx.
11. Values match: Test CACIE-ModelSetupFY18.jar-AT-3, Test Steps 4.1 to 4.2(as described in Table A-4 below) passed.
12. Compared input.bot (output from CAST) to calculated values in compare\_input\_bot.xlsx.
13. Values match: Test CACIE-ModelSetupFY18.jar-AT-3, Test Steps 5.1 to 5.2(as described in Table A-4 below) passed.
14. Copied side-by-side comparison between input (output from CAST) and the CAST input pages into input\_comparison.pptx and checked values.
15. Values match: Test CACIE-ModelSetupFY18.jar-AT-3, Test Steps 6.1 to 6.16 (as described in Table A-4 below) passed.

**Tool Runner Log:**

INFO--02/03/2020 04:41:26 PM--Starting CA-CIE Tool Runner. Logging to "./runner\_CAST\_test\_logfile.txt"

INFO--02/03/2020 04:41:26 PM--Invoking: Command:"python" Arguments:"S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\fingerprint\fingerprint.py ..\..\CA-CIE-Tools-Testing\tools\CAST\ModelSetupFY18.jar --output .\fingerprint\_ModelSetupFY18.jar.txt"

INFO--02/03/2020 04:41:28 PM--Code Version: 1f1673849bd63b1795ee57fe48b0a237a91663d6 v1.1: S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\runner\runner.py

INFO--02/03/2020 04:41:29 PM--Code Version: 1f1673849bd63b1795ee57fe48b0a237a91663d6 v1.1: S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\fingerprint\fingerprint.py

INFO--02/03/2020 04:41:31 PM--QA Status: QUALIFIED : S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\runner\runner.py

INFO--02/03/2020 04:41:32 PM--QA Status: QUALIFIED : S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\fingerprint\fingerprint.py

INFO--02/03/2020 04:41:32 PM--Username:dfryar Computer:PSC-Sodium Platform:Windows 10 10.0.18362

INFO--02/03/2020 04:41:34 PM--Starting CA-CIE Tool Runner. Logging to "./runner\_CAST\_test\_logfile.txt"

INFO--02/03/2020 04:41:34 PM--Invoking: Command:"java" Arguments:"-Dsun.java2d.dpiaware=false -jar -Djava.library.path=..\..\CA-CIE-Tools-Testing\tools\CAST\lib -Xmx7000m -Xms7000m ..\..\CA-CIE-Tools-Testing\tools\CAST\ModelSetupFY18.jar"

INFO--02/03/2020 04:41:35 PM--Code Version: ecd17a8b08df3aea37edf1d043b18dfd1fbbf53c Local repo SHA-1 has does not correspond to a remote repo release version: ..\..\CA-CIE-Tools-Testing\tools\CAST\ModelSetupFY18.jar

INFO--02/03/2020 04:41:37 PM--Code Version: 1f1673849bd63b1795ee57fe48b0a237a91663d6 v1.1: S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\runner\runner.py

INFO--02/03/2020 04:41:38 PM--Code Version: ecd17a8b08df3aea37edf1d043b18dfd1fbbf53c Local repo SHA-1 has does not correspond to a remote repo release version: ..\..\CA-CIE-Tools-Testing\tools\CAST\lib

INFO--02/03/2020 04:41:39 PM--QA Status: TEST : ..\..\CA-CIE-Tools-Testing\tools\CAST\ModelSetupFY18.jar

INFO--02/03/2020 04:41:40 PM--QA Status: QUALIFIED : S:\PSC\!HANFORD\ICF\CA-CIE-Tools\CA-CIE-Tools\pylib\runner\runner.py

INFO--02/03/2020 04:41:41 PM--QA Status: TEST : ..\..\CA-CIE-Tools-Testing\tools\CAST\lib

INFO--02/03/2020 04:41:41 PM--Username:dfryar Computer:PSC-Sodium Platform:Windows 10 10.0.18362

| **Table A-1**  **CAST Acceptance Test Case Plan 1** | | | |
| --- | --- | --- | --- |
| **CAST Installation or Acceptance Testing**  **CACIE-ModelSetupFY18.jar-AT-1 Building the Model Grid** | | **Date: 02-03-2020** | |
| **Tool Runner File Location for this test:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST\build](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST\build) | | **Test Performed By: Dennis Fryar** | |
| **Testing Directory:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST)\buildTool runs in Windows | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| Navigate to the Testing Directory | | | | |
| 1 | Invoke Tool runner and test the tool using:  *runner\_run\_AT-1\_CAST.bat* | CAST GUI loads. | **Pass** |
| **Screenshot of the Tool Runner executed for this test.**  Text file present in the testing directory. | | | | | |
| 2 | Click on *acceptancetest1-mdef.xml* under Available Model Definition Files and click on the Revise button. | File is loaded. | **Pass** |
| 3 | In the Simulation Builder window revise the following fields:   * User Name: Insert your full first and last name * Organization/Company: Intera, Inc. * Title: Composite Analysis (CA) * Simulation Description:   + First line “Acceptance Test1”   Second line should read “Steady-State Simulation,” | Details are correctly input in the Simulation Builder window. | **Pass** |
| 4 | Click on the Grid button under the Simulation Categories to open the Finite Difference Grid Builder window | Opens up the Finite Difference Grid Builder window. | **Pass** | |
| 5 | In the STOMP Grid section be sure the following are selected:   * Grid Type: Cartesian * Elevation button * Specification: Manual | Values selected/input. | **Pass** |
| 6 | Under the X Surfaces section:   * Units: m * Definition Option: CSV   List Points: 567400,2@50,2@40,1@20,80@10,1@20,2@40,2@50 | Values selected/input. | **Pass** | |
| 7 | Under the Y Surfaces section:   * Units: m * Definition Option: CSV   List Points: 135500,2@40,1@20,50@10,1@20,2@40 | Values selected/input. | **Pass** | |
| 8 | Under the Z Surfaces section:   * Units: m * Definition Option: CSV   List Points: 126.9, 195@0.5 | Values selected/input. | **Pass** | |
| 9 | Click Exit in the Finite Difference Builder window. | Window closes. | **Pass** | |
| 10 | Click Save in the Numerical Model Setup window, type in your name, and click OK to save the changes. | *\*-mdef.xml* File is saved. | **Pass** | |
| 11 | Click on *acceptancetest1-mdef.xml* under Available Model Definition Files and click on the Revise button. Click Material Mapping | Opens the Material Mapping window. | **Pass** | |
| 12 | Click the Generate LeadFrog File button to open the window Generate LeapFrog File (XYZ CSV).  Input the file name as *test1.csv* and click OK. | Generates the *test1.csv* in the directory. | **Pass** | |
| 13 | Click OK.  Click Exit.  Click Save in the Numerical Model Setup window, type in your name, and click OK to save the changes. | *\*-mdef.xml* File is saved. | **Pass** | |
| 14 | Outside of CAST, create a file to calculate the node centers of each node within the model domain. Use the X, Y, and Z gridding from above.  This file will be titled and referred to as *calculated-nodes.\**, where the \* could be “xlsx” or any other user chosen file type. | A separated calculation file is created. | **Pass** | |
| 15 | Compare the separate calculation file against the *test1.csv* file generated from CAST. | The two files match for each node center and the total number of nodes. | **Pass** | |
| 16 | Proceed to CACIE-ModelSetupFY18.jar-AT-2. | | | |

| **Table A-2**  **CAST Acceptance Test Case Plan 2** | | | |
| --- | --- | --- | --- |
| **CAST Installation or Acceptance Testing**  **CACIE-ModelSetupFY18.jar-AT-2 Material Mapping Generation** | | **Date: 02-03-2020** | |
| **Tool Runner File Location for this test:**  [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST\build](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST\build) | | **Test Performed By: Dennis Fryar** | |
| **Testing Directory:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST)\buildTool runs in Windows | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| 1 | If you closed CAST after CACIE-ModelSetupFY18.jar-AT-1 then repeat steps 1 through 2 of CACIE-ModelSetupFY18.jar-AT-1. | The configuration file is loaded. | **Pass** | |
| 2 | Click on Material Mapping | Opens the Material Mapping window. | **Pass** |
| 3 | In the Material Mapping section enter in the File Name: *test1-eval.csv* | File name is typed in. | **Pass** |
| 4 | Click Scan File for Codes at the base of the Material Mapping window | Read the eval file & populate the File Material Mapping section with two columns of data, Material Name and Code in File. | **Pass** |
| 5 | The Material Name cells will need to be selected based on the associated cell present in the Code in File column.   1. For Air the Material Name will be Inactive 2. For Surface Deposits the Material Name will be Backfill   For the rest of the units, the Material Name matches the Code in File. |  | **Pass** |
| 6 | Click the Preview button at the top of the Material Mapping window. | This will take a few moments to generate a separate window, Grid View, showing a three-dimensional representation of the grid and geology currently mapped. | **Pass** | |
| 8 | Adjust the depth exaggeration to 10. | Subsurface is more visible. | **Pass** | |
| 9 | Confirm that the top of the model grid has at least a single grid cell of the top-most geologic unit (typically Backfill) present.  The geology looks appropriate for your model domain | User verifies at least one grid node present at uppermost layer. | **Pass** | |
| 10 | Close the Grid View window. | Window closes. | **Pass** | |
| 11 | Exit the Material Mapping window. | Window closes. | **Pass** | |
| 12 | Click Save in the Numerical Model Setup window. | Saves. | **Pass** | |
| 13 | Open Model Definition Selection window. | Window opens. | **Pass** | |
| 14 | Select the model name you wish to create input files for, the *acceptancetest1-mdef.xml* in the File Name column under the Available Model Definition Files section. |  | **Pass** | |
| 15 | Click the Generate Simulator Input File button at the bottom of the window. | Window opens. | **Pass** | |
| 16 | Press OK with the default file name, input. | This will take several minutes.  The following output text will be generated in the command shell window when complete:  “Simulation Input File Build Completed Successfully at: [date/time]”. | **Pass** | |
| 17 | In the build the folder the following files will be generated | input,  input.buildLog,  input.zone,  input.sij,  input.nij,  input.top,  input.bot,  input.north,  input.south,  input.west,  input.east | **Pass** | |

| **Table A-3**  **CAST Acceptance Test Case Plan 3** | | | |
| --- | --- | --- | --- |
| **CAST Installation or Acceptance Testing**  **CACIE-ModelSetupFY18.jar-AT-3**  **Verify Files Generated by CAST** | | **Date: 02-04-2020** | |
| **Tool Runner File Location for this test:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST\build](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST\build) | | **Test Performed By: Dennis Fryar** | |
| **Testing Directory:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST)\buildTool runs in Windows | | | |
| **Test Step** | **Test Instruction** | **Expected Result** | **Test Result  (Pass/Fail)** |
| 1 | Navigate to the Testing Directory, where the files from the final step of CACIE-ModelSetupFY18.jar-TC-2 were generated. | | |
| 1.1 | **Verify the *input.zone* file**  Node material numbers/values in the *input.zone* file should match material types in the Kingdom2Stomp output file, *test1-eval.csv*.  Using the input.zone file and the grid definition (~Grid Card) and material definitions (~Rock/Soil Zonation Card) in the input file, create a file listing X, Y, Z and material type (corresponding to the zone number in the input.zone file) for each model node. | File containing calculated X, Y, Z and material type for each model node | **Pass** |
| 1.2 | Compare this file against the *test1-eval.csv* file. | Files match. | **Pass** |
| 2.1 | **Verify the *input.sij* file**  Calculate node surface coordinates for X and Y (i.e., model plan view). The file should include surface count in the i-direction, surface count in the j‑direction, X and Y for each model node corner in plan view. | File containing plan view node corner locations | **Pass** |
| 2.2 | Compare *input.sij* to the calculated node corner locations to verify the files match | All lines in the files match. | **Pass** |
| 3.1 | **Verify the *input.nij* file**  Calculate node center coordinates for X and Y (i.e., model plan view). The file should include node count in the i-direction, node count in the j‑direction, X and Y for each model node center in plan view. | File containing plan view node center locations. | **Pass** |
| 3.2 | Compare *input.nij* to the calculated node center locations to verify the files match | All nodes in the files match. | **Pass** |
| 4.1 | **Verify the *input.top* file**  Ensure the file contains the top surface of the uppermost active node in each ‘ij’ column.  Using the input.zone file and the grid definition (~Grid Card) and material definitions (~Rock/Soil Zonation Card) in the input file, create a file listing i, j, k and material type (corresponding to the zone number in the input.zone file) for each model node. From this file, determine the uppermost active node in each ij column. | Uppermost active nodes are calculated. | **Pass** |
| 4.2 | Compare *input.top* to the calculated uppermost active node in each ij column to verify the files match. | All nodes in the files match. | **Pass** |
| 5.1 | **Verify the *input.bot* file**  Ensure the file contains the bottom surface plane nodes in each ij column.  Calculate bottom node for each ij column. The file should include node i, j, k and surface number for the bottom, | Bottom layer of nodes are calculated. | **Pass** |
| 5.2 | Compare *input.bot* to the calculated bottom node in each ij column to verify the files match. | All nodes in the files match. | **Pass** |
| 6 | Open the *input* file and begin the verification process below. | | |
| 6.1 | **~Simulation Title Card**  Check that information in the ~Simulation Title Card matches entries in the Numerical Model Setup - Simulation Builder section of CAST | Matches. | **Pass** |
| 6.2 | **~Solution Control Card**  Check that information in the ~Solution Control Card matches entries on the CAST Simulation Controls page (selected from Numerical Model Setup page). | Matches. | **Pass** |
| 6.3 | **~Grid Card**  Check that information in the ~Grid Card matches entries on the CAST Finite Difference Grid Builder page (selected from Numerical Model Setup page). | Matches. | **Pass** |
| 6.4 | **~Inactive Nodes Card**  Check that the *input.zone* zonation file is referenced. | Is referenced. | **Pass** |
| 6.5 | **~Rock/Soil Zonation Card**   * Check that the *input.zone* zonation file is referenced * Check that the material types listed in the *~Rock/Soil Zonation Card* match entries in the *Material Name* list (excluding Inactive) on the CAST Material Mapping page (selected from Numerical Model Setup page). | Is referenced & matches. | **Pass** |
| 6.6 | **~Mechanical Properties Card**  Check that information in the ~Mechanical Properties Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. | **Pass** |
| 6.7 | **~Hydraulic Properties Card**  Check that information in the ~Hydraulic Properties Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. | **Pass** |
| 6.8 | **~Saturation Function Card**  Check that information in the ~Saturation Function Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. | **Pass** |
| 6.9 | **~X-Aqueous Relative Permeability Card**  Check that information in the ~X-Aqueous Relative Permeability Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. | **Pass** |
| 6.10 | **~Y-Aqueous Relative Permeability Card**  Check that information in the ~Y-Aqueous Relative Permeability Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. | **Pass** |
| 6.11 | **~Z-Aqueous Relative Permeability Card**  Check that information in the ~Z-Aqueous Relative Permeability Card matches entries on the CAST Material Properties page (selected from Numerical Model Setup page). Values for each material type are accessed by selecting the Material Name and then Revise. | Matches. | **Pass** |
| 6.12 | **~Initial Conditions Card**  Check that information in the ~Initial Conditions Card matches entries on the CAST Initial Conditions page (selected from Numerical Model Setup page). | Matches. | **Pass** |
| 6.13 | **~Boundary Conditions Card**  Check that information in the ~Boundary Conditions Card matches entries on the CAST Boundary Conditions page (selected from Numerical Model Setup page). Typically, for the steady-state models there are no boundary conditions. | Matches. | **Pass** |
| 6.14 | **~Source Card**  Check that information in the ~Source Card matches entries on the CAST Sources/Sinks page (selected from Numerical Model Setup page). typically, for the steady-state models there are no sources or sinks. | Matches. | **Pass** |
| 6.15 | **~Output Control Card**  Check that information in the ~Output Control Card matches entries on the CAST Output Specifications page (selected from Numerical Model Setup page). | Matches. | **Pass** |
| 6.16 | **~Surface Flux Card**  Check that information in the ~Surface Flux Card matches entries on the CAST Output Specifications page, Surface Flux tab (selected from Numerical Model Setup page). | Matches. | **Pass** |

**Appendix B**

**Installation Test Logs**

|  |  |  |  |
| --- | --- | --- | --- |
| **Table B-1**  **CAST Installation Test Plan** | | | |
| **CAST Installation Testing**  **CACIE-ModelSetupFY18.jar-IT-1** | | **Date:** | |
| **Tool Runner File Location for this test:** | | **Test Performed By:** | |
| **Testing Directory:** [\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2\_CAST](file:///\\olive\cfarrow\CAVE\CA-CIE-Tools-TestEnv\v4-2_CAST) Tool runs in Windows | | | |
| **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 cast using .bat file using below command:  *./runner\_run\_IT-1\_CAST.bat* | | |
| 2 | Verify Tool Runner is invoked and executed. | Tool runner file is generated.  Cast GUI interface is loaded. |  |
| 3 | Close the terminal window used to execute Tool Runner. | Window closes. |  |