1. eSTOMP Software Test Plan, Rev. 1.1 2
1.1 1.0 Introduction to STP 2
1.2 2.0 Limitations 3
1.3 3.0 Test Identification 5
1.4 4.0 Test Results Archival and Documentation 7

eSTOMP Software Test Plan, Rev. 1.1

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Approvals

This document is electronically approved and signed via the PNNL Electronic Records & Information Capture Architecture (ERICA) system.

Revision History

Revision	Date	Summary of Changes
1.0	02/2015	Original Version
1.1	05/2016	clarified that testing includes a subset of all options

1.0 Introduction to STP

This document describes the software test plan (STP) for eSTOMP, the scalable version of Subsurface Transport Over Multiple Phase (STOMP) software used to support work under a number of different environmental assessments. This plan also includes pre- and post-processing utilities used in conjunction with eSTOMP. Post-processors for eSTOMP are written in Perl. The pre-processor *toEcke* and eSTOMP are written in FORTRAN90.

1.1 Purpose

This document provides information on the requirements and procedures necessary for testing eSTOMP software in support

of changes made in accordance with the eSTOMP Software Configuration Management Plan (SCMP).

This STP identifies specific tests to be run for two separate purposes. First, the tests will help ensure that the eSTOMP modules are correctly performing their intended function. Second, this plan identifies a standard suite of tests to be performed when software changes are made. Initially all tests in this test plan will be executed. Subsequently, only the specific modules being modified under an approved Software Change Request (SCR) will require testing to ensure the changes are implemented as desired. If changes made could affect other modules, then regression testing will be performed.

1.2 Definitions

Term	Definition
DOE	Department of Energy
SVN	Subversion (configuration management software)
PNNL	Pacific Northwest National Laboratory
PIC	PNNL Institutional Computing (Program responsible for maintaining High Performance Computing Clusters)
RL	Revision Log
SCM	Software Configuration Manager
SCMP	Software Configuration Management Plan
SCR	Software Change Request
eSTOMP	Scalable version of Subsurface Transport Over Multiple Phases
STP	Software Test Plan

1.3 References

- STOMP SharePoint (https://spcollab.pnnl.gov/sites/stompshare/SitePages/Home.aspx)
- STOMP Software Requirements Document (SRD)

2.0 Limitations

The eSTOMP simulator has been written with a variable source code that allows the user to choose the solved governing equations (e.g., water mass, air mass, salt mass, thermal energy, CO_2 gas). Depending on the chosen operational mode, the governing transport equations will be written over different phases.

In addition to the variable source code configuration, separate branches of eSTOMP source code are maintained. Production versions of eSTOMP are isolated from the research branch of the code. Currently, the only qualified version of eSTOMP is the -W and -W-R modes. This qualified version of eSTOMP is termed NQA-1.

Due to the complexity of the variable source code configuration, eSTOMP testing has been divided into three different stages, and is based on a thorough testing of the primary operational mode of water.

1. In the first stage of testing, basic functionality of the operational mode is tested, using a limited number of options. In addition to testing for the operational mode's intended functions, unintended uses are also tested. This first stage of testing is executed on only one processor using the serial STOMP test suite. Results from eSTOMP are verified against serial STOMP results.
2. In the second stage, eSTOMP is executed on multiple processors and these results are compared with the serial results for eSTOMP that were verified in the first stage of testing.
3. In the third stage of testing, larger test problems designed for execution on high performance machines will be tested

for both results verification and performance.

eSTOMP Operational Modes

Operational Mode Name	Operational Mode Identifier
STOMP-W[a]	Water
STOMP-WAE[b]	Water-Air-Energy
STOMP-CO2e	Water-CO_2-Energy

a Can also be executed with ECKEChem Reactive Transport Module (-R)
b Can also be executed with Barrier (Plant) Module (-B)

2.1 Software Test Plan Maintenance

This plan will remain in effect as long as PNNL is supporting assessments with the eSTOMP software, or further use of the software is contemplated. The SCM will have responsibility to monitor compliance, and ensure that changes and updates are reflected in the STP, as required. Reviews of this STP will occur periodically throughout the project's life. Revisions to this STP will be managed manually, per the SCMP. This STP will be stored on the STOMP SharePoint site, and in draft form on the internal PNNL Confluence website in the eSTOMP space.

End use testing will be conducted before releasing source code to verify that any changes in the software, hardware and/or operating system have not impacted results. Test problems, are accessible on the STOMP/eSTOMP SharePoint under the appropriate subdirectory as categorized by simulator and operational mode. This activity is documented in the appropriate test logs.

2.2 Software Test Environment

Currently, eSTOMP testing is carried out on PNNL Institutional Computer (PIC) clusters, which run UNIX Linux-based operating systems. PIC supports large-scale clusters of multiprocessor supercomputers, special purpose testbeds, databases, web servers, and application frameworks. To date, eSTOMP testing is performed on olympus.pnl.gov, but may also be performed on constance.pnl.gov (another PIC supported cluster) in the future. eSTOMP results are verified by comparing them to serial STOMP, whose results have been verified against analytical solutions. STOMP tests are also run on a UNIX Linux-based system, but have been executed on a RedHat workstation (PC). PIC is a continuously changing R&D environment hence, any potential issues that may arise from running in this type of environment are mitigated by the direct comparison of STOMP and eSTOMP results, since test problem solutions are known a priori. For example, if results from the eSTOMP tests do not match those from STOMP, then the tester and development team can immediately identify if updates to the OS were the root cause.

The development environment is also a Linux-based system (e.g., RedHat workstations, PIC). Software is compiled using the Intel compiler for both development and regression testing. When eSTOMP software is checked out of the SVN repository for testing, the tester will compile the source code and create an executable for testing. Once the executable is compiled, the tester removes write (-w) permissions for all users (including the owner) of that directory. This is to protect the integrity of the source code and executable that reside within that directory.

Testing is performed by eSTOMP users, as assigned by the SCM. The SCM may also perform testing. eSTOMP developers may be used for testing, as long as the tests they perform are not code that they have developed. Although developers are responsible for testing, independent testing will be performed before the new source is accepted for production. A log file of results will be generated from each new test and its location recorded in PNNL's JIRA tracking system. If only component testing is required, then the comparison to previous results will be recorded in JIRA. However, for code that was checked into the repository before FY14 (before the current management plan was put into place), there is no tracking system that accompanies source code updates and identify the locations of the test logs, as eSTOMP was developed using internal research funds (LDRD). Results of eSTOMP testing will be archived in SVN and posted to the STOMP/eSTOMP SharePoint site.

3.0 Test Identification

The software modes and scripts that will be tested as part of this test plan are identified by name in the table below. A brief description of each software module and script is provided, as well as the tests required for configuration control. In the sections that follow, the tests planned for the software and scripts are described, and follow the requirements outlined in the eSTOMP SRD requirements document.

In general, most of the testing outlined in this document will be component testing, and will be structured to evaluate the correctness of the code. System-level (regression) testing will only be carried out on the source code for new source releases. The results of that testing will be recorded in JIRA. Complete automation of the testing process has been established. Analytical solutions will be used to verify test results when possible. In the absence of analytical solutions, experimental data may also be used to verify results.

Name	Program Description	Test Description
eSTOMP-W	Water flow and solute transport (and ECKEChem)	Compare numerical unsaturated and saturated flow results executed on a single processor to serial STOMP results.
eSTOMP-WAE	Water flow and solute, air and energy transport (and with barrier)	Compare numerical unsaturated and saturated flow results e xecuted on a single processorto serial STOMP results.
eSTOMP-CO2/CO2e	Water flow and solute, carbon and salt transport (and ECKECHEM)	Compare numerical unsaturated and saturated flow results e xecuted on a single processorto serial STOMP results.

Multiple processor runs were compared to eSTOMP runs executed on a single processor.

3.1 eSTOMP Utilities

Perl utilities can be used to extract data from STOMP and eSTOMP output files to formatted output for Tecplot, Gnuplot, Igor and Grapher. Current testing focuses on verifying output for Tecplot and Gnuplot, since Igor and Grapher are not commonly used at PNNL. These scripts are maintained and tested under the serial STOMP Configuration Management Plan.

3.2 Acceptance Criteria

It is expected that differences between the serial STOMP solution and the parallel eSTOMP solution will occur due to differences in the library used for solving the governing equations. When eSTOMP is executed on a single processor, this error is expected to be small, and should be no greater than 1%. As the number of processors increases, the multi-processor solution can diverge even further from the serial solution. However, differences no greater than 3% are anticipated for the primary variables. It is anticipated, however, that this error (~10%) may be larger in cases for very small numbers (e.g., 10^{-14} or smaller).

Once a baseline has been established for the tests, testing will be automated and results compared to the archived results. An exact match should occur between the new and archived results, but if the solutions differ by less than 1%, this may also be acceptable if the tester and/or developer can identify a reasonable cause for these differences (e.g., change in compiler, operating system, etc.). Any acceptable differences will be used to establish a new baseline for future testing.

3.3 eSTOMP

eSTOMP testing is carried out on an operational mode basis (as identified in the eSTOMP SRD). For each operational mode, a base case is established that tests its basic functionality. This base case is stored under the *base* subdirectory of the

operational mode that is being tested. In the water mode, for example, a base case is stored under *stomp-w/base*. A second base case is stored under *stomp-w-t/base* that tests the functionality of solute transport. Because testing is structured on operational modes that have already been tested, only one base case may exist for other operational modes.

Once a base case test has been established, different options are tested, although this is a subset of the total number of options available in the code. Tested options are identified in both the User Guide and Software Requirements Document. These options are grouped by type, as organized by the input structure. For example, options in the water mode (eSTOMP-W) include several different tests of boundary conditions, which are tested under the *bc* subdirectory. The different options that are tested exist in numbered subdirectories, and the correspondence of the numbered directory to the option being tested is recorded in an external database. Boundary condition options also exist for solute transport (eSTOMP-W-T), and exist in a separate subdirectory under the estomp-w-t directory. The table below shows how testing is structured, and mimics the directory structure used to carry out both the component and system level tests.

For modes that consider other phases, testing is focused on the functionality of each phase in that mode. For example, in the water mode with geochemical transport, testing of the water phase is carried out in the e*stomp-w-r*directory.

Operational Mode	Sub-directory	Description
eSTOMP-W (flow)	base	base case
	arp	aqueous relative permeability
	bc	boundary conditions
	gc	grid card
	hp	hydraulic properties
	ic	initial conditions
	in	inactive nodes
	mp	mechanical properties
	oc	output control
	rsz	rock/soil zonation
	sc	solution control
	sf	saturation function
	sfl	surface flux
	src	source card
	st	simulation title
	unintended	unintended uses
eSTOMP-W (transport)		
	base	base case
	bc	boundary conditions
	ic	initial conditions
	oc	output control
	sc	solution control
	sfi	solute fluid interactions
	sfl	surface flux

	spm	solute porous medium
	src	source card
	unintended	unintended uses
eSTOMP-W-R (geochemisty)		
	distKd	spatially variable Valochi sorption model
	phreeqc	phreeqc benchmark (ftp://brrftp.cr.usgs.gov/pub/dlpark/geochem/unix/phreeqc/manual.pdf)
	glass	ILAW glass simulation
	reducedChem	The reduced chemistry formulation
	seawater	Pitzer activity is equivalent to PHREEQC calculations for seawater using Pitzer activity model.
	ionex	http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/index.html.
	LowpH	precipitation/dissolution w/bufffering

Once a capability in the code has been verified by the appropriate test, these tests will be used as a baseline for future tests. Test problems that are relevant to the mode that has been changed will be executed to ensure that new bugs are not introduced. Regression test results will be performed for new releases of eSTOMP and documented in JIRA. These tests will also be traced to their related software requirements.

The test suite for eSTOMP will be automated to the extent possible through the use of Cmake, shell scripts and batch submission scripts, and the results compared to the previously verified results. If results do not match, the root cause of the discrepancies will be identified. All discrepancies and their cause will be documented in the SCR and/or test log.

4.0 Test Results Archival and Documentation

A clear, documented history of test results is necessary to build confidence that all software and scripts maintain integrity during the development cycle. This section specifies requirements and procedures for documenting test results.

The SCM is responsible for ensuring that all tests for software and scripts are conducted and properly documented. Test problems or information about test problems will be located on the STOMP/eSTOMP SharePoint. The test problems directory will be subdivided into subdirectories, as defined previously in this document.

All software and script documentation (e.g., bug fixes, new source code features) will be maintained in the JIRA repository tracking system and in SCR forms stored on the STOMP SharePoint.

Test logs also briefly describe program functions, and necessary input and output files. The initial verification of all source codes or scripts maintained by the SCM will be documented in JIRA. Test logs that are output from the use of the Cmake utility are stored in the eSTOMP SVN repository under a branch called *testing*. Tables are also maintained on the SharePoint site that describe each of the test cases, the expected results, the metrics used for testing, and the date the tests were successfully completed.

The STOMP SharePoint is backed up and maintained by PNNL and is therefore not managed by the eSTOMP team.