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STOMP Software Test Plan
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Revision Log

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Approvals

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1.0 Introduction

This document describes the software test plan for the Subsurface Transport Over Multiple Phase (STOMP) software used to support work under a number of different environmental assessments. The software test plan also includes pre- and post-processing utilities used in conjunction with STOMP.

1.1 Purpose

This Software Test Plan provides information on the requirements and procedures necessary for testing STOMP software in support of changes made in accordance with the STOMP Software Configuration Management Plan.

This Software Test Plan identifies specific tests to be run for two separate purposes. First, the tests will help ensure that the STOMP 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 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

Glossary

Term	Definition
DOE	Department of Energy
CVS	Concurrent Versions System (configuration management software)
NAPL	Non-Aqueous Phase Liquid
PNNL	Pacific Northwest National Laboratory
RL	Revision Log
SCM	Software Configuration Manager
SCR	Software Change Request
STOMP	Subsurface Transport Over Multiple Phases
STP	Software Test Plan

1.3 Limitations

The STOMP 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, dissolved-oil mass, oil mass, salt mass, thermal energy, CO_2 gas). Depending on the chosen operational mode, the governing transport equations will be written over one to four phases (e.g., aqueous phase, gas phase, (nonaqueous phase liquid) NAPL phase, ice phase, solid phase). In addition to the variable source code configuration, two separate sources of STOMP are maintained. The primary STOMP source code is in FORTRAN77 and may be executed only on a single processor. The second STOMP source is written in FORTRAN90, and is designed for execution on multiple

processors. This scalable version of STOMP90 is only available in select operational modes, and contains only a subset of the options available in STOMP77. Only the FORTRAN77 version of STOMP is distributed to users outside the Pacific Northwest National Laboratory (PNNL). The scalable version of STOMP is only available to internal users. STOMP modes currently in production are listed in Table 1.1. The scalable version of STOMP is denoted with a -*SC*.

Due to the complexity of the variable source code configuration, STOMP testing has been divided into three different stages, and is based on a thorough testing of the primary operational mode of water. 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. In the second stage, options for the non-water modes are tested for both intended and unintended uses. For example, the second stage of STOMP-WO involves only testing the options describing oil transport. In the third stage of testing, water options for the operational mode are tested. Although these options have been tested in the STOMP-W mode, different subroutines are accessed in different operational modes. Hence, testing is required for governing equations that have already been tested in other operational modes.

The initial testing of the different operational modes is prioritized based on the need for compliance with the Department of Energy (DOE) order 414.1.C. STOMP operational modes that are currently used in DOE safety software applications are tested before operational modes that are not currently being applied with that same classification.

Table 1.1 STOMP Operational Modes

MODE	Governing Equations
STOMP-W	Water
STOMP-W-SC	Water (scalable)
STOMP-WS	Water and Salt
STOMP-W-R	Water with Reactions
STOMP-WA	Water and Air
STOMP-WO	Water and Oil
STOMP-WOA	Water, Oil and Air
STOMP-WOA-SC	Water, Oil and Air (scalable)
STOMP-WAE	Water, Air and Energy
STOMP-WAE-B	Water, Air and Energy with Barrier
STOMP-WCS	Water, CO_2 and Salt
STOMP-WCS	Water, CO_2 and Salt (scalable)
STOMP-WCS-R	Water, CO_2 and Salt with Reactions
STOMP-WCSE	Water, CO_2, Salt and Energy
STOMP-WCMSE	Water, CO_2, Methane, Salt and Energy

1.4 Software Test Plan Maintenance

This Software Test Plan will remain in effect as long as PNNL is supporting assessments with the STOMP software, or further use of the software is contemplated. The Software Configuration Manager will have responsibility to monitor compliance, and ensure that changes and updates are reflected in the Software Test Plan, as required. Reviews of this Software Test Plan will occur periodically throughout the project's life.

Revisions to this Software Test Plan (STP) will be managed manually as follows. The document is written in Microsoft Word. To modify the STP, a copy will be made of the current version. In the copy, all changes in the prior version recorded using Word's Track Changes feature will be accepted, and the Track Changes feature used to record new changes for the revision. The STP document will include the new version number in the file name. Version numbering will be in the form x.x, with increments in the first number made if the revision includes changes to procedures, requirements, or software tests, and increments in the second number made if the changes are editorial. The most current version of this STP will be stored in agua:/files0/STOMP-QA/docs/software_test_plan/ in Linux, and all older versions in agua:/files0/STOMP-QA/docs/software_test_plan/archive/.

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 at agua:/files0/STOMP-QA/stomp-tests / under the appropriate subdirectory as categorized by operational mode. This activity is documented in the appropriate test logs.

1.5 Software Test Environment

The software and scripts listed in Table 1.2 are executed in a UNIX Linux-based system. The development environment is also a Linux-based system, but is based on the Mac OS. Software is compiled using the Portland Group compiler for both development and testing. Post-processors for STOMP are written in Perl. Testing is done by STOMP users, as assigned by the SCM. The SCM may also perform testing. STOMP 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 test and its location recorded on the Change Implementation section of the Software Change Request (SCR). However, for code that was checked into the repository before FY07 (before the current management plan was put into place), there are no SCRs that accompany source code updates and identify the locations of the test logs. Test logs will be generated and archived on agua in the test directory corresponding to the mode and input card deck.

1.6 Test Identification

The software modes and scripts that will be tested as part of this test plan are identified by name in Table 1.2. 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 STOMP requirements document (Zhang, 2007).

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 a Revision Log. Complete automation of the testing process will be executed once the initial verification of software and scripts 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.

1.6.1 STOMP77

STOMP testing is carried out on an operational mode basis. 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. For example, only one base case exists for STOMP-WA that tests the basic functionality of air transport.

Once a base case test has been established, different options are tested. These options are grouped by type, as required by the input structure. For example, options in the water mode (stomp-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 conditions options also exist for solute transport (stomp-w-t), and exist in a separate subdirectory under the stomp-w-t directory. Table 1.3 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-air mode (STOMP-WA), testing of the water phase is carried out in the *stomp-wa-w* directory, and testing of the air phase is carried out in the *stomp-wa-a* directory.

Table 1.2 STOMP Modes and Post-Processors

MODE/ Script Name	Program Description	Test Description	Testing Targets	Target Completion Dates
STOMP77 MODES Requiring Immediate Compliance with 414.1.C				
STOMP-W	Water flow and solute transport	Compare numerical unsaturated and saturated flow results to analytical solutions	STOMP-W Base	03/01/07
			STOMP-W Options	
			STOMP-W-T Base	
			STOMP-W-T Options	
STOMP-W-R	Water flow, solute transport, and multicomponent reactive transport	Compare numerical results of flow to analytical solutions; Compare reactive chemical transport to results generated from USGS reaction code, PHREEQC	STOMP-W-R Base	03/01/07
			STOMP-W-R Options	Funding Not Yet Identified
STOMP-WA	Water flow and solute and air transport	Compare numerical results of flow and air transport to analytical solutions	STOMP-WA-W Base	03/01/07
			STOMP-WA-W Options	
			STOMP-WA-T Base	
			STOMP-WA-T Options	
			STOMP-WA-A Base	
			STOMP-WA-A Options	
STOMP-WAE	Water flow and solute, air and energy transport	Compare numerical results of flow and energy and air transport to analytical solutions	STOMP-WAE Base	03/01/07
			STOMP-WAE Options	Funding Not Yet Identified
			STOMP-WAE-T Base	03/01/07
			STOMP-WAE-T Options	Funding Not Yet Identified
STOMP-WAE-B	Water flow and solute, air and energy transport with a barrier	Compare numerical results of flow to analytical solutions; Compare energy transport to field data; Compare numerical results of air transport to analytical solutions	STOMP-WAE-B Base	03/01/07
			STOMP-WAE-B Options	Funding Not Yet Identified
			STOMP-WAE-B-T Base	03/01/07

MODE/ Script Name	Program Description	Test Description	Testing Targets	Target Completion Dates
			STOMP-WAE-B-T Options	Funding Not Yet Identified
STOMP-W-RO	Water flow and solute and oil transport	Compare numerical results of flow and NAPL transport to analytical solutions	STOMP-WO Base	03/01/07
			STOMP-WO Options	Funding Not Yet Identified
			STOMP-WO-T Base	03/01/07
			STOMP-WO-T Options	Funding Not Yet Identified
STOMP-WOA	Water flow and solute, oil and air transport	Compare numerical results of flow and NAPL and air transport to analytical solutions	STOMP-WOA Base	03/01/07
			STOMP-WOA Options	Funding Not Yet Identified
			STOMP-WOA-T Base	03/01/07
			STOMP-WOA-T Options	Funding Not Yet Identified
STOMP-WCS	Water flow and solute, carbon and salt transport	Compare numerical results of flow and CO_2 and salt transport to analytical solutions	STOMP-WCS Base	Funding Not Yet Identified
			STOMP-WCS Options	
			STOMP-WCS-T Base	
			STOMP-WCS-T Options	
STOMP-WCS-R	Water flow and solute, carbon and salt transport with multicomponent reactive transport	Compare numerical results of CO_2 and salt transport to analytical solutions; Compare reactive chemical transport to results generated from USGS reaction code, PHREEQC	STOMP-WCS-R Base	Funding Not Yet Identified
			STOMP-WCS-R Options	
			STOMP-WCS-R-T Base	
			STOMP-WCS-R-T Options	
STOMP-WCSE	Water flow with solute, carbon, salt and energy transport	Compare numerical results of flow and CO_2, energy and salt transport to analytical solutions	STOMP-WCSE-R Base	Funding Not Yet Identified
			STOMP-WCSE-R Options	
			STOMP-WCSE-R-T Base	

MODE/ Script Name	Program Description	Test Description	Testing Targets	Target Completion Dates
			STOMP-WCSE-R-T Options	
STOMP-WCMSE	Water flow with solute, carbon, methane, salt and energy transport	Compare numerical results of flow and CO_2, methane, energy and salt transport to analytical solutions	STOMP-WCMSE-R Base	Funding Not Yet Identified
			STOMP-WCMSE-R Options	
			STOMP-WCMSE-R-T Base	
			STOMP-WCMSE-R-T Options	
Other STOMP77 MODEs				
STOMP-WS	Water flow with solute and salt transport	Compare numerical results salt transport to analytical solutions		Funding Not Yet Identified
STOMP77 MODEs Under Development				
STOMP-WA-R	Water flow with solute and air transport with equilibrium and kinetic chemical reactions	Compare numerical results of air transport to analytical solutions; Compare reactive chemical transport to results generated from USGS reaction code, PHREEQC		Currently Under develop-ment
STOMP-WO-R	Water flow with solute and air transport with multicomponent reactive transport	Compare numerical results of NAPL transport to analytical solutions; Compare reactive chemical transport to results generated from USGS reaction code, PHREEQC		Currently Under develop-ment
STOMP-WOA-R	Water flow with solute, oil and air transport with multicomponent reactive transport	Compare numerical results of NAPL and air transport to analytical solutions; Compare reactive chemical transport to results generated from USGS reaction code, PHREEQC		Currently Under develop-ment
STOMP-WCASE	Water flow with solute, carbon, air, salt and energy transport	Compare numerical results of CO_2, air, energy and salt transport to analytical solutions		Currently Under develop-ment
STOMP90 MODEs Requiring Immediate Compliance with 414.1.C				

MODE/ Script Name	Program Description	Test Description	Testing Targets	Target Completion Dates
STOMP-W-SC	Water flow with solute transport	Compare results of scalable version to results generated by STOMP77 (non-scalable STOMP)	STOMP-W-SC Base STOMP-W-SC Options STOMP-W-SC-T Base STOMP-W-SC-T Options	03/01/07
STOMP-WCS-SC	Water flow with solute, carbon and salt transport	Compare results of scalable version to results generated by STOMP77 (non-scalable STOMP)	STOMP-WCS-SC Base STOMP-WCS-SC Options STOMP-WCS-SC-T Base STOMP-WCS-SC-T Options	Funding Not yet identified
STOMP90 MODEs Under Development				
STOMP-WAE-B-SC	Water flow and solute, air and energy transport with a barrier	Compare results of scalable version to results generated by STOMP77 (non-scalable STOMP)		Currently Under develop-ment
STOMP-WAE-B-R-SC	Water flow and solute, air, energy and multicomponent reactive transport with a barrier	Compare results of scalable version to results generated by STOMP77 (non-scalable STOMP)		Currently Under develop-ment
STOMP Utilities				
plotTo.pl	Utility for converting STOMP plot file output to formatted output for Tecplot, Gnuplot, Igor and Grapher	Compare plot file output to results generated by Perl script	N/A	03/01/07
surfaceTo.pl	Utility for converting STOMP surface file output to formatted output for Tecplot, Gnuplot, Igor and Grapher	Compare surface file output to results generated by Perl script	N/A	03/01/07
outputTo.pl	Utility for converting STOMP output file to formatted output for Tecplot, Gnuplot, Igor and Grapher	Compare output file to results generated by Perl script	N/A	03/01/07

MODE/ Script Name	Program Description	Test Description	Testing Targets	Target Completion Dates
biogeoTo.pl	Utility for converting geochemical preprocessor output to input format suitable for STOMP ECKECHEM	Compare input data to reformatted output	N/A	03/01/07
tecplot.F90	Utility for converting STOMP90 binary plot file output to formatted output for Tecplot	Implicitly tested when comparing scalable STOMP results to STOMP77, since this program extracts binary plot file output to Tecplot formatted files	N/A	03/01/07

Table 1.3 STOMP-W Tests/Directory Structure

Operational Mode	STOMP Input Card/Subirectory	Description
STOMP-W		
	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
STOMP-W-T		
	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

Analytical solutions are used to verify STOMP solutions whenever possible. In the absence of analytical solutions, data is used to verify the numerical solution. For some options, like the inactive nodes, rock/soil zonation and solution control cards, only the input read is confirmed and no comparison to alternative solutions is necessary.

1.6.2 STOMP90 (Scalable)

Since a non-scalable version of each of the STOMP90 modes exist, the STOMP77 tests will be used to verify the solutions for all STOMP-SC(alable) modes. Because STOMP-SC is run on multiple processors, some divergence of results is expected due to differences in compilers, operating system and execution on multiple processors, but results should not differ by more than 1%.

1.6.3 STOMP Utilities

Perl utilities can be used to extract data from STOMP77 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.

1.7 Acceptance Criteria

It is expected that differences between the analytical and numerical results will occur due to numerical error in the STOMP solution. This error can be minimized with grid discretization and time stepping control schemes such that the difference between analytical and numerical solutions is no greater than 3%. It is anticipated, however, that this error (~10%) may be larger for air transport, given that the volume of the air being transported is much smaller than other phases that predominate (e.g. water). This is especially relevant for numbers that are close to the precision of the calculation (e.g., 10^{-14} or smaller), where large differences (up to a couple of orders of magnitude) are acceptable.

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.

1.8 Test Schedule

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 tests will be performed for new releases of STOMP and documented in a Revision Log (RL).

The test suite for STOMP77 will be automated through the use of C shell scripts, and the results compared to the previously verified results. Because jobs need to be submitted individually on the supercomputer for the scalable version of STOMP, the regression testing cannot be automated with the use of C shell scripts, and will need to be executed individually. 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.

2.0 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 Software Control Manager (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 in the agua:/files0/STOMP-QA/stomp-tests/ directory. This directory is not accessible through Windows, but only on Linux through the Hydronet. The test problems directory will be subdivided into subdirectories, as categorized in Table 1.3.

All software and script documentation (e.g., bug fixes, new source code features) will be maintained in the CVS repository tracking system and in Software Change Request (SCR) forms stored in agua:/files0/STOMP-QA//SCRs directory. Documentation of STOMP90 is described in the STOMP user and theory guides (White and Oostrom 2006; White and Oostrom 2000). 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 with test logs that are archived in the options subdirectories in each of the operational modes. Test logs that follow the initial baseline testing of the source code will be archived in the *verify_logs* subdirectory of the operational mode.

The agua directories are backed up every day to hard disk. These backups are incremental, only backing up changes that have occurred since the last full backup. Full backups are done on the first day of every month. When a new version of the source code is released all source pertaining to the new release are to be written to tape. A one-month retention period for all data is maintained.

3.0 References

White M.D. and M. Oostrom. 2006. STOMP Subsurface Transport Over Multiple Phases Version 4.0: User's Guide. PNNL-15782, Pacific Northwest National Laboratory, Richland, Washington.

White, M.D., and M. Oostrom. 2000. STOMP Subsurface Transport Over Multiple Phase: Theory Guide PNNL-11216 (UC-2010), Pacific Northwest National Laboratory, Richland, Washington.