QA: QA

SOFTWARE ACTIVITY PLAN (SAP)
for
TOUGHREACT Version 2.2

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PRELIMINARY DRAFT
INFORMATION ONLY

CHANGE HISTORY

Revision Number	Effective Date	Description of Change
00	03/15/00	Initial issue of CP1 documents prior to ITSMA review. Previously, a SAP was submitted and a Software Activity Number was issued under Section 5.12 of AP-SI.1Q, Rev. 2, ICN 2.
01	05/1/00	Initial issue of CP1 documents following ITSMA review. The changes were the addition of the "QA" designator, this Change History, changes to the appendix to include referenced material and the resulting change in page numbers.

I. WORK SCOPE, OBJECTIVES, AND PRIMARY TASKS

Work Scope

This work is performed under YMP Analysis/Model Report (AMR) U0110, *Drift-Scale Coupled Processes (DST, THC Seepage) Models* TDP-NBS-HS-000007. The LBNL work is covered under Master Planning Document (MPD) YMP-MPD-UZ-1.0, *UZ Flow and Transport Modeling FY99*, Section 1. The interfaces with primary organizations for this work is given in the MPD, Section 14. The specific tasks and responsibilities of the individuals responsible for this work are given below under "Primary Tasks" (see Attachment A for MPD sections).

TOUGHREACT V2.2 has a previous Software Activity Plan (SAP) under Section 5.12 of AP-SI.1Q, Rev. 2, ICN 2, *Software Management,* for use of unqualified software. In accordance with AP-SI.1Q, Rev.2, ICN 4, this SAP, 10154-SAP-2.2-01 is part of the qualification effort and is followed by Requirements Document (RD), 10154-RD-2.2-01.

In accordance with AP-SI.1Q, Rev. 2, ICN 4, Subsection 5.2, the centralized baseline was checked and no suitable software was found. Therefore, the objectives and primary tasks were formulated as listed below.

Objectives

TOUGHREACT V2.2 will be upgraded from TOUGHREACT V2.1 (STN: 10042-2.1-01), which has already been qualified (Spycher et al. 1999). The main upgrades in V2.2, from V2.1, will consist of:

1. All upgrades necessary for consistency with TOUGH2 EOS3 v1.4 (STN: 10007-1.4-01) (Wu et al. 1999): active-fracture model, downstream weighting option, capillary pressure linear extrapolation at low liquid saturations, changes in relative permeability based on a modified Brooks-Corey model;
2. Restart option for reactive transport;
3. New option for calculating gas diffusion coefficients as function of temperature and pressure;
4. Use input tortuosity to weight molecular diffusion coefficients;
5. New options for calculating effective surface areas;
6. New option for precipitation rate law;
7. Time dependent thermal conductivity factors;
8. New conjugate gradient stabilized solver;
9. Carmen-Kozeny porosity-permeability coupling option;
10. Modified output options and formats (separate plot ouput file for gases, option to output gas and mineral amounts in volume fraction, output additional variables such as porosity and permeability in plot files).

Primary Tasks

The PI responsible for this task is Eric Sonnenthal. Under his direction, Nicolas Spycher will perform the specific tasks of coding and testing. The primary task is to develop TOUGHREACT V2.2 with the capabilities listed under "Objectives" above.

II. SCHEDULES

The proposed schedule for qualification and baselining is given in the table below.

Life Cycle Phase	*Proposed Completion Date*
Functional Requirements	3/09/00
Design	3/10/00
Control Point 1 Review	3/13/00
Implementation	3/11/00
Validation	3/11/00
Control Point 2 Review	3/13/00
Final Release for Use	3/14/00

III. SCIENTIFIC APPROACH OR TECHNICAL METHODS

The general scientific approach and technical methods are listed in Section I and in the MPD, Section 2 (Attachment A).

Procedures to be followed as necessary are the current versions of:

- AP-SI.1Q, *Software Management*
- YMP-LBNL-QIP-SIII.0, *Scientific Investigation* (prior to 9/17/99), and AP-SIII.1Q, *Scientific Notebook* (after 9/17/99)
- AP-3.10Q, *Analyses and Models*
- AP-3.15Q, *Managing of Technical Inputs*
- AP-2.14Q, *Reviews of Technical Products* (for external reviewers of AMRs)
- YMP-LBNL-QIP-6.1, *Document Review* (for internal reviews)

Compliance will be assured by the technical, management, and Information Technology Software Management Analyst (ITSMA) reviews mandated by these procedures.

IV. STANDARDS AND CRITERIA

FORTRAN77 is to be used for coding. No additional or external standards or criteria to Section III above are to be imposed or implemented within this software activity.

V. IMPLEMENTING DOCUMENTS

See Section III above for YMP and LBNL procedures. For software usage, scientific notebooks are employed.

VI. EQUIPMENT

Not applicable as no laboratory or field equipment is to be employed.

VII. RECORDS

The records that are identified in the procedures listed in Section III above (with the exception of AP-SI.1Q) will be created and submitted to the Records Processing Center (RPC) in accordance with AP-17.1Q, *Record Source Responsibilities for Inclusionary Records.* Records associated

with AP-SI.1Q will be transmitted to the Software Configuration Secretariat (SCS) for submittal to the RPC.

- AP-SI.1Q, *Software Management*;
  - ♦ Completed Software Baseline Request (SBR)
  - ♦ Documentation regarding software recommendation and software selection
  - ♦ Control Point 1 documentation:
    - Software Activity Plan (SAP)
    - Requirements Document (RD)
    - Design Document (DD)
    - Installation Test Plan (ITP)
    - Validation Test Plan (VTP)
  - ♦ Control Point 2 documentation:
    - The appropriate software media [source code, object code, or executable, as applicable]
    - Users Manual (UM)
    - Validation Test Report (VTR)
  - ♦ Documentation of regression testing, as applicable

VIII. INDEPENDENT AND IT SOFTWARE REVIEWS

No additional independent, management, or Information Technology (IT) reviews are planned for Control Points 1 and 2 other than those mandated by the current revision of AP-SI.1Q.

IX. PREREQUISITES

No prerequisites, special controls, environmental conditions, processes, or special skills are required for this planned software development activity. No In-use testing is not planned for this software because the standard means of testing are sufficient.

X. ERROR REPORTING AND CORRECTIVE ACTION

The error reporting and corrective action process of the current revision of AP-SI.1Q, will be followed.

References:

CRWMS M&O 1999. *Coupled Processes (DST, THC Seepage) Models.* ANL-NBS-HS-000006 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL 19990721.0523.

Spycher, N., Sonnenthal, E., Ahlers, R., and Xu, T., *TOUGHREACT V2.1 Software Qualification*, 1999. MOL.20000216.0113.

Wu, Y.S., Haukwa, C., and Mukhopadyay, S., *TOUGH2 V1.4 and T2R3D V1.4: Verification and Validation Report and User's Manual,* Rev 00, 1999. MOL 20000216.0111

APPENDIX A Excerpts from YMP-MPD-UZ-1.0, UZ Flow and Transport and Modeling FY99

1. OBJECTIVES, WORK SCOPE, AND PRIMARY TASKS

1.1 Objectives

The purpose of this work is to continue the development and application of the Unsaturated Zone (UZ) Site Scale Flow and Transport Model (UZ Model) and develop a defensible model for Site Recommendation (SR) and License Application (LA) by:

- updating the model grid,
- updating calibrated property sets based on recently available data and refining the calibration process,
- further evaluating conceptual models of flow and transport,
- evaluating ambient geochemistry transport from the land surface to the water table,
- predicting conditions at the repository horizon and water table including the spatial percolation flux, water vapor migration, and the thermal regime,
- performing limited simulations of coupled thermal-hydrologic (TH) and thermal-hydrologic-chemical (THC) processes to determine the effect on flow and transport, and
- providing support to PA in performing abstractions from the UZ Model.

1.2 Work Scope

See Attachment 1 for the work scope as documented in the TRW/Civil Radioactive Waste Management System (CRWMS) Management and Operations (M&O) Contractor, Lawrence Berkeley National Laboratory (LBNL) FY99 Statement of Work, Revision 4, LV.SS.TSP.09/98-403, dated 3/29/99. Revision 5 of the work scope has not been issued as of the effective date of this MPD. Revision 5 or a later revision will include the cancellation of deliverables SP3538M4 and SPB177M5 under WP 14012027M2 and SPB176M4 under WP 14012027M3. This MPD reflects the expected changes to be incorporated in Revision 5 or a later revision of the work scope. It should also be noted that the funding level for this work has not been finalized, and therefore certain tasks (as identified in Section 1.3) may not be completed in FY99.

1.3 Primary Tasks

14012027M2 - UZ Site Scale & Transport Model-SR-FY99

Task 1. *Update Model* - Incorporate all relevant hydrologic, thermal, geochemical, pneumatic and isotopic data including new site data from Busted Butte, PTn, Niche studies, ESF Main Drift, and ECRB. Develop fully-integrated conceptual model incorporating all site data and occurrences of perched water.

- Update fracture properties using fracture mapping data from the ECRB
- Reevaluate matrix properties (saturation, porosity, permeability) by utilizing data from original core measurements
- Reevaluate fault properties using data from Ghost Dance Fault, when available

- Evaluate at least two different conceptual models for perched water

Task 2. *Refined Model Gridding and 1-D Inversions for Calibrated Property Set* - Refine model grid for better representation of spatial resolution of infiltration flux; incorporate most recent Geologic Framework Model (GFM); and revise calibrated hydrological property set to incorporate new site data using Calibrated Properties Model.

- Design refined grid based on FY98 grid
- Update grid using new GFM
- Update mineralogy in grid using Integrated Site Model (ISM)
- Evaluate effects of grid discretization on flow
- Evaluate effects of grid discretization on transport
- Use site data to estimate fracture and matrix properties for input into the Calibrated Properties Model
- Perform 1-D inversions using the Calibrated Properties Model, calibrating matrix and fracture properties to pneumatic pressures, saturations, and potentials.
- Develop base case calibrated hydrological property set based on 1-D inversions for deliverable SP3540M4.
- Perform forward calibrations on temperature data
- Perform forward calibrations using alternative perched water conceptual models
- Develop revised base case calibrated hydrological property set based on forward calibrations

Task 3. *Percolation to Depth Simulations and Ambient Geochemistry with PA Transport Module* - Perform simulations of percolation to the repository horizon and the water table and provide predictions of the ambient geochemistry from the land surface to the water table.

- Evaluate alternative conceptual models
- Evaluate alternative fracture/matrix interaction approaches
- Perform simulations using UZ Model to determine percolation to depth using base case calibrated property set
- Evaluate impact of future climate change on percolation
- Perform forward calibrations on geochemical data using the UZ Model
- Perform forward calibrations on tracer data, if available
- Reevaluate calibrated flow and transport property sets

Task 4. *Configuration Control for TOUGH2, Quality Assurance, Information Transfer, Model Documentation, and Summary Report* - Maintain internal configuration management controls for site-scale and drift-scale codes; meet standards for data reviews and reports; submit data to the Technical Database Management System (TDMS); prepare documentation for the site-scale model; and initiate work on comprehensive document summarizing work.

- Implement software configuration management controls

- Submit data to the TDMS per YMP-LBNL-QIP-SIII.3 Submitting Key Data to the Yucca Mountain Project Office and YAP-SIII.3Q Processing of Technical Data on the Yucca Mountain Site Characterization Project
- Document all models, submodels, and analyses per AP-3.10Q Analyses and Models.
- Review deliverables, reports and corresponding scientific notebooks per YMP-LBNL-QIP-6.1 Document Review

Task 5. *Limited[*] Modeling of Mountain-Scale TH and THC Processes and Durable Changes in Rock Properties* - Model mountain-scale reaction-transport processes for nonisothermal multicomponent, multiphase, multispecies systems. These models will combine constraints and data from the modeling of ambient system geochemistry and coupled processes in the thermal tests, including constraints on reaction rates from isotopic systems, such as strontium and carbon. Utilize the Mountain-Scale Thermal-Hydrology (TH) Model and the Mountain-Scale Thermal-Hydrologic-Chemical (THC) Model.

- Evaluate efficiency of code for TH simulations
- Reevaluate TH property sets and conceptual models
- Perform limited simulations using the Mountain-Scale TH Model to evaluate the impact of repository heat on water and gas flow.
- Perform limited simulations using the Mountain-Scale THC Model to estimate hydrologic property changes, water chemistry changes, and mineral dissolution / precipitation due to repository heat.

Task 6. *Advection-Dispersion Flow & Transport Confirmation* – Simulate radionuclide transport using a fully coupled advective dispersion flow and transport model that incorporates advection, dispersion, sorption, and decay processes. Results will be compared with TSPA particle tracking results.

- Perform simulations using TOUGH2 modules T2R3D and EOS9nT for comparison to particle tracking results completed for TSPA Viability Assessment
- Resolve differences, if any, between results

Task 7. *Limited[*] Modeling of Radionuclide Transport* - Perform simulations of transport of radionuclides from the repository horizon to the water table as needed to support model development and support studies for PA.

14012027M3 - UZ Abstraction Testing-SR-FY99

The following tasks will be performed under this work package:

- Provide technical and consultative support (including scoping analyses, prioritization of cases, and problem domain setup) to PA for specific activities related to abstraction of UZ Flow and Transport Model.
- Participate in PA process model abstraction workshops

[*] The funding level for this task has not been finalized, and therefore all, some or none of this task will be completed in FY99.

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- Provide follow-up support to PA for activities determined at workshops

2. SCIENTIFIC APPROACH OR TECHNICAL METHODS

Dual permeability (DKM) and effective continuum (ECM) approaches will be used for modeling flow processes in unsaturated fractured and porous media. In general, the UZ Model will be used to model flow and transport. It utilizes the software code TOUGH2. TOUGH2 is a second generation version of the TOUGH simulator ("transport of unsaturated groundwater and heat"). It is a multi-dimensional numerical model for simulating the coupled transport of water, vapor, non-condensible gas, and heat in porous and fractured media. TOUGH2 uses an integral finite difference method for space discretization, and first-order fully implicit time differencing. A sparse direct solver or various preconditioned conjugate gradient algorithms can be used for linear equation solutions. Thermophysical properties of water are represented by steam table equations provided by the International Formulation Committee.

Property sets for model grid layers will be developed using the Calibrated Properties Model. This will include both inversions utilizing the code ITOUGH2 and forward calibrations using the UZ Model. The Mountain-Scale TH and THC Models will be used to simulate coupled heat and flow processes and coupled geochemical, heat and flow processes, respectively. These models utilize the codes TOUGH2 and TOUGHREACT, respectively. The modules T2R3D, EOS9nT, and EOS7nR (modules of TOUGH2) will be used for modeling of radionuclide transport.

14. COORDINATION WITH OUTSIDE ORGANIZATIONS AND AGENCIES

Input data used for this work will be retrieved from the TDMS. In addition, new data from the following studies will be used (once available from the TDMS) to update the model and perform calibrations:

- Geologic Framework Model (GFM)
- Integrated Site Model (ISM)
- ECRB Fracture Mapping
- Infiltration Model
- Ghost Dance Fault Data Package
- Perched Water Age Data
- Sr Isotopic Data
- Geochemical Data from X-Drift
- Hydrologic Parameters for Busted Butte
- Transport Data from Busted Butte
- Fracture-Mineral Age Data from ESF
- ESF Moisture Monitoring Data

- Alcove 1 Experimental Results
- Niche Seepage Data
- Colloid Lab and Modeling Data
- Colloid Formation Parameters
- Colloids Modeling Results
- Additional Sorption Data
- Drift Scale Test Data Feeds

Los Alamos National Laboratory (LANL) will be completing a task entitled *Enhanced Colloid Transport Process Description* under this same work package. LANL will develop a defensible model for colloid transport by performing 1-D and 2-D modeling studies for incorporation into the PA Colloids Abstraction Model. LANL will also review and provide comments regarding the work completed in Tasks 1 and 3 under WP 14012027M2.