

QA: QA

**SOFTWARE ACTIVITY PLAN
FOR USE OF UNQUALIFIED VERSION OF
TOUGHREACT V2.2**

Software Activity Number: LBNL-1999-141

Software Tracking Number: 10154-2.2-00

January 21, 2000

The purpose of this Software Activity Plan (SAP) is to comply with requirements in AP-SI.1Q Rev. 2, ICN 2 (*Software Management*), for use of unqualified software. Section 5.12 in that procedure details the requirements, which include the issuance of this SAP. Note that this SAP is specific to the use of unqualified software, and it complements any existing SAP associated with the Software Activity Number and Software Tracking Number identified above.

1. WORK SCOPE, OBJECTIVES, AND PRIMARY TASKS

The scope of this work includes performing simulations of thermal loading conditions and fracture-matrix interactions through the unsaturated zone (UZ), in support of the UZ PMR that in turn supports the Site Recommendation (SR). The objective of these simulations is to provide insight to the nonisothermal geochemical reactions in the UZ Model. The primary task includes calculations of geochemistry under thermal loading for the UZ Model. The work is performed with TOUGHREACT V2.2, which is currently being qualified per AP-SI.1Q.

Eric Sonnenthal or a designee at Lawrence Berkeley National Laboratory (LBNL) will perform the initial simulations and the verification runs described below.

2. SCHEDULES

The qualification of TOUGHREACT V2.2 is expected to be completed by mid-February 2000. At that time, the simulations that were run using the unqualified version will be re-run using the qualified version and compared to the original runs by the beginning of March 2000. Documentation, revisions, and impact reviews (if required) will be completed by the end of March 2000.

<i>Life Cycle Phase</i>	<i>Proposed Completion Date</i>
Functional Requirements	2/1/00
Design	2/2/00
Control Point 1 Review	2/4/00
Implementation	2/8/00
Validation	2/9/00
Control Point 2 Review	2/10/00
Final Release for Use	2/11/00

3. SCIENTIFIC APPROACH OR TECHNICAL METHODS

The scientific method in this activity is to use the currently unqualified numerical code TOUGHREACT V2.2 to study nonisothermal geochemical reactions in the UZ. The simulation approach is described in more detail in Analysis/Model Report (AMR) U0110 *Drift-Scale Coupled Processes (DST, THC Seepage) Models* (CRWMS M&O 2000).

After TOUGHREACT V2.2 is qualified, a suite of comparison runs will be performed to verify the results produced by the unqualified version of the code. Representative simulations will be re-run using the qualified version, and results will be directly compared with the unqualified results using visual inspection of key output variable values. The acceptance criteria is to have the same (numerical) output within rounding up to 3 significant figures. Results shall be documented in Rev 01 of AMR U0050 *Coupled Processes (DST, THC Seepage) Models* (CRWMS M&O 2000). If any output variable values do not meet the acceptance criteria, any corrections necessary will be made to the code and affected documentation, and the need for an impact analysis will be assessed. If needed, an impact analysis will be performed per AP-3.17Q (*Impact Reviews*).

4. STANDARDS AND CRITERIA

There are no applicable standards and criteria for this activity, other than the acceptance criteria mentioned in paragraph 3.

5. IMPLEMENTING DOCUMENTS

In addition to AP-SI.1Q, AP-3.17Q will be invoked if impact analyses are found to be necessary. AP-3.10Q will be used in activities related to the use of this software for the AMR.

6. EQUIPMENT

No additional equipment is required to perform this work other than standard office equipment such as computers, telephones, etc.

7. RECORDS

The records identified in Sections 5.12 and Section 6.0 of AP-SI.1Q will be submitted as part of this activity.

8. INDEPENDENT AND QUALITY ASSURANCE VERIFICATIONS

No additional verifications or reviews are required in addition to those outlined in AP-SI.1Q.

9. PREREQUISITES

The prerequisites for this task include familiarity with the code TOUGHREACT V2.2.

10. ERROR REPORTING AND CORRECTIVE ACTION

No additional methods for error reporting or corrective action are required in addition to those outlined in AP-SI.1Q.

REFERENCES

AP-SI.1Q, Rev. 2, ICN 2. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19991214.0627.

AP-3.10Q, Rev. 1, ICN 1. *Analysis and Models*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990702.0314.

AP-3.17Q, Rev. 0, ICN 0. *Impact Reviews*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990702.0306.

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.

**OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SOFTWARE USER REQUEST**

QA: QA

Complete Only Applicable Items

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1. Software Activity Number: LBNL-1999-141	2. Software Name and Version: TOUGHREACT V2.2	3. Software Tracking Number: 10154-2.2-00
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4. Organizational and geographical location where software will be used:
NW/ESD, Lawrence Berkeley National Laboratory, Berkeley, CA

5. Central Processing Unit (CPU) Number(s) (property tag number(s) or CPU serial number(s):
6332537

6. State the intended use of the software in the new environment:
Use TOUGHREACT V2.2 for analysis and modeling of nonisothermal multiphase flow, transport, and mineral-water reactions under kinetic and/or equilibrium conditions on workstations with Unix.
CD, diskette, or FTP methods may be used to transfer files.

6b. <input checked="" type="checkbox"/> Distribute Software to a Single Computer	6c. <input checked="" type="checkbox"/> Server Access <input checked="" type="checkbox"/> Single Access <input checked="" type="checkbox"/> Read <input type="checkbox"/> Write <input type="checkbox"/> Multiple (Global) Access <input type="checkbox"/> Read <input type="checkbox"/> Write
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7. List of users who are qualified to use the software and will have access to the CPU(s):
Eric Sonnenthal, Nick Spycher, Tianfu Xu, Jianchun Liu

8a. Responsible Manager Name: G. S. Bodvarsson	8b. Responsible Manager Org.: NW/ESD/LBNL	8c. Date 1/21/00
8d. Responsible Manager Telephone Number: 510-486-4789	8e. Responsible Manager Facsimile Number: 510-486-6115	

9a. Software Configuration Secretariat Name: Greg Carlisle	9b. Date: 01/24/00
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10. Installation/Reinstallation Successful. Software operating as expected.
 Installer Name: _____ Initials: _____ Date: _____