

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

CORRECTIVE ACTION REQUEST

CAR No: 2004-1

Associated AR, SR, NCR No: SR 2004-5, -11 NCR 2004-04

PART A: DESCRIPTION OF CONDITION ADVERSE TO QUALITY

Contrary to the CNWRA Quality Assurance Manual, Section 3.3.5, uncontrolled software (software not under TOP-018 control) has been used in the development of CNWRA technical products.

1. Report - *Chemical Speciation Using Thermodynamic Modeling During a Representative Loss of Coolant Accident Event - Draft Report*, June 29, 2004 includes a reference to Stream Analyzer, Version 1.2 and Environmental Simulation Program, Version 6.6. Stream Analyzer, Version 1.2 and Environmental Simulation Program, Version 6.6 were placed under TOP-018 configuration control after release of the report.
2. Report - *Final Report on Experiments to Model Normal Faulting in Carbonate Strata Above Salt Domes and 3D Digital Fault analysis to Estimate Synthetic Fracture Network of Zakum Field*, June 2004 includes a reference to FracWorks XP, version Beta 0.22. FracWorks XP, version Beta 0.22 is not under TOP-018 control.
3. Report - *MECHFAIL: A Total-system Performance Assessment Code Module for Evaluating Engineered Barrier Performance Under Mechanical Loading Conditions*, April 28, 2003 (Revision 1) includes a reference to HyperMesh, Version 3.1. HyperMesh, Version 3.1 was not under TOP-018 controls when the report was released. This issue was resolved via NCR 2004-04.

Initiated by: R. Folck
Date July 12, 2004

Responsible Individual: B. Sagar
Response Due: August 6, 2004

PART B: PROPOSED ACTION

1) Extent of Condition: To determine the extent of condition, all CNWRA reports produced since January 1, 2004 to date were checked. Twenty reports identified software use. In addition to the three reports identified in Part A above, four more reports were found to have used unqualified software. In three of these cases, the software used was a more recent version of previously qualified commercial software. In the fourth case, a version of MCNP was used that was identified in the 'Master Directory of Software' as 'will not be used in regulatory reviews'. Attached Table 1 shows the analyses of the three violations recorded in Part A and Table 2 shows the four cases discussed here. Considering that 7 out of 20 reports used unqualified software prompted a more extensive analysis of the extent of condition. Reports produced in CY 2003 were evaluated, and it was determined that no report produced that year used unqualified software.

Each of the reports using unqualified software included a statement on the Acknowledgment page incorrectly indicating that the used software were qualified.

2) Root Cause: Technical investigators did ^{not} confirm the qualification status of the software before use. Contributing factor: Managers and reviewers did not verify software status during the document review process.

3) Remedial Action: Proposed Completion Date: September 6, 2004

The uncontrolled software identified in the investigation (Tables 1 and 2) will be placed under TOP-018 control. If any acceptance test results suggest that errors may have occurred affecting technical reports, the analyses shall be repeated with controlled software and if necessary, the reports shall be revised and resubmitted to the client.

4) Corrective Action to Preclude Recurrence: Proposed Completion Date: September 1, 2004

- (a) Revise QAP-013 (Quality Planning) to require that the qualification status of software be verified when the software is expected to be used in the task.
- (b) Maintain the Master Directory of Scientific and Engineering Software on the QA website for improved, universal access to the most current version of the directory. Revise the directory to clearly distinguish between qualified software and retired or restricted use software.
- (c) Revise QAP-002 (CNWRA review process) to (1) require that managers verify software status when authors present documents for review, (2) specify that technical reviewers verify software status and validation range (e.g., by examination of the applicable scientific notebook or other objective evidence), and (3) include a software qualification status check.

Element Manager/Director: *Burclii Sagar*

Date: *7-22-2004*

PART C: APPROVAL

Comments/Instructions
Director of QA: *R. Folck*

Date: *7/23/2004*

PART D: VERIFICATION OF CORRECTIVE ACTION IMPLEMENTATION

See attached

Distribution:
Original-CNWRA/QA DIRECTOR QA Records
ORIGINATOR: R. Folck
PRINCIPAL INVESTIGATOR
MANAGER
TECHNICAL DIRECTOR
CNWRA PRESIDENT

Verified by: *R. Folck*

Date: *11/11/2004*

extended to 9/20/04
extended to 10/1/2004
9/21/04
10/15/04

Table 1: Analysis of Uncontrolled Software Use - CAR 2004-1

Report	Report Acknowledgment Statement	GRAM Statement	Discussion
Chemical Speciation Using Thermodynamic Modeling During a Representative LOCA Event ...	"Stream Analyzer 1.2 and Environmental Simulation Program 6.6 are controlled per TOP-018"	"OLI Systems software are already under TOP-018 control."	Report and GRAM had incorrect statements. These code versions had been validated in December 2003, but TOP-018 control was not completed. Previous versions were under control. Remedial action has been completed.
Final Experiments on Normal Faulting ... (Japan National Oil Co.)	None in acknowledgment. Report text indicates FracWorksXP was used to create synthetic fracture networks. No statement of qualification status.	FracWorks not mentioned in GRAM	This was probably an oversight - staff assumed FracWorksXP had been placed under control. No remedial action has been taken.
MECHFAL Report	"Hypermesh 3.1 is controlled per TOP-018."	Hypermesh was not listed in the GRAM	Acknowledgment statement is incorrect. Versions 4 and 5 had been controlled prior to this report, not sure why an earlier version (3.1) was used. Remedial action taken per NCR 2004-4.

Table 2: Extent of Condition Analysis for CAR 2004-1

Sample: 11 reports dated 1/1/2004 through 7/14/2004 were identified as using software. Unqualified software was identified as follows (these are in addition to the three instances cited in CAR 2004-1):

Report	Report Date	Unqualified Code Used
Preliminary Evaluation and Analysis of U.S. DOE Geotechnical Data for the Waste Handling Building Site at the potential Yucca Mountain Repository	6/2004	Earthvision 7.0.1 was used, only versions 5.0.1 and 5.1 are controlled. Report acknowledgment claimed that the software was under TOP-018 control.
Dose Assessment for Compliance with the Radiological Criteria for License Termination at the Dow Chemical Company Site at Bay City, Michigan	5/2004	PHREEQC V. 2.8 was used, however version 2.6 is qualified. Report acknowledgment claimed that the software was under TOP-018 control.
Idaho Spent Fuel Facility Safety Evaluation Report	4/2004, 1/2004	MCNP 4C2 and 4B2 were used in this regulatory review. 4C2 is validation category IV, (not to be used for regulatory reviews). Versions 5 and 4A are under TOP-018 control in category II. 4B2 is not under TOP-018.
Thermally Induced Rock Stress and Implications for Degradation of Emplacement Drifts at the Potential Yucca Mountain, Nevada Waste Repository	4/2004	ABAQUS V.6.3 was used, however, only versions 6.2 and 5.8-16 are under TOP-018 control. Report acknowledgment claimed that the software was under TOP-018 control.

Close out of CAR 2004-1

1. Remedial action:

The following software was placed under control:

Earthvision version 7	8/31/2004	
PHREEQC version 2.8	9/8/2004	
ABAQUS version 6.3	8/2/2004	
FRACMAN (including FRACWORKS) version 2.606		8/4/2004

MCNP version 4C2 was determined to be exempt from validation. see the attached memo.
MCNP 4B2 was not used in the subject report.

2. Corrective Action to Preclude Recurrence:

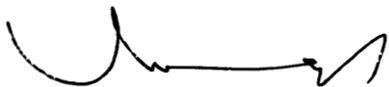
- a. QAP-013 was revised to incorporate the specified changes on 8/10/2004 (Revision 7).
- b. The master directory of controlled software is available on tutu\QA and on the shared G: drive.
- c. QAP-002 was revised to incorporate the specified changes on 8/13/2004 (Revision 9, change 1)

Note to CAR 2004-1 File:

MCNP version 4C2 was identified in CAR 2004-1 as having been used in a regulatory review without having been validated. Remedial action specified for MCNP 4C2 was to validate this version. Upon further investigation, the staff noted that MCNP is identified in NUREG 1536, Standard Review Plan for Dry Storage Casks, as appropriate for use in shielding analysis. NUREG 1536 was identified in the regulatory review report (for the Idaho Spent Fuel Facility) as being applicable.

Since MCNP is designated by the NRC for use in the type of analysis performed in the subject report, MCNP should be considered to be valid for this application. Note also that TOP-018, Revision 9 (currently in draft) includes a provision for accepting NRC endorsement (or designation) in lieu of validation. Therefore, the disposition of the use of MCNP 4C2 should be changed to "Accept as is" and the basis is NRC endorsement of MCNP for the subject application.

Asadul H. Chowdhury



Manager; Mining, Geotechnical, and
Facility Engineering.

11-11-2004



Director of Quality Assurance

11-11-2004

Date