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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

CORRECTIVE ACTION REQUEST

CAR No: 96-03

Associated AR, SR, NCR No: CNWSA AR 96-01

PART A: DESCRIPTION OF CONDITION ADVERSE TO QUALITY

QAP-001, Para. 3.3 defines initial and in-process entries as providing documentation of planning, experimental design, methods, and equipment (initial) and specific conduct of the technical activities and results. (See attached.)

Initiated by: Donald W. Dunavant *DWB*

Date: 7/26/96

PART B: PROPOSED ACTION

Responsible EM: **E. Percy**
Response Due: **8/15/96**

1) Extent of Condition: **See attached.**

2) Root Cause: **See attached.**

3) Remedial Action: **See attached.**

Proposed Completion Date: *11/1/96*

4) Corrective Action to Preclude Recurrence: **See attached.**

Proposed Completion Date: *9/20/96*

Element Manager:

E. C. Percy

Date:

8/27/96

PART C: APPROVAL Comments/Instructions

*Reviewed and discussed with Center QA
DWB 9/1/96*

Director of QA:

Shun Malenko

Date:

8/29/96

PART D: VERIFICATION OF CORRECTIVE ACTION IMPLEMENTATION

*SEE April 18, 1997 Memo To CAR 96-03.
CORRECTIVE ACTIONS AND REMEDIAL ACTIONS
HAVE BEEN COMPLETED.*

Distribution: **E. Percy**
B. Sagar
W. Patrick

Verified by:

Shun Malenko

Date:

4/28/97

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Contrary to the above requirements, a number of scientific notebooks evaluated during the course of the audit were deficient in describing the planning, objectives, methods, or results such that there was a high confidence that another qualified individual might understand and/or repeat the activity.

Examples were scientific notebooks covering such activities as development of code for MULTI-FLO, development of calculational methods for preliminary calculations of expected dose from volcanism, and notebooks associated with field sample collection and code evaluation for near field investigation. Notebooks included # 164, 121, 140, 180, 185.

Proposed Action:

1) **Extent of Condition:** Since the audit evaluated five of the ten KTIs and found "a number of" the Scientific Notebooks deficient, the condition appears sufficiently extensive so that remedial and preventive action is necessary for many active notebooks and affected technical staff.

2) **Root Cause:** The shift in program direction away from research projects has resulted in a greater portion of code development and analysis work in comparison to laboratory and field investigations. The use of Scientific Notebooks for code development and analysis is not nearly so obvious and routine as it is for laboratory and field investigations. As a result, the staff have not implemented Scientific Notebook controls as effectively for this type of activity.

3) **Remedial Action:** The passage of time precludes accurately supplementing past notebook entries with additional detail. However, existing notebooks shall be brought back into compliance from this point on by providing new initial entries in accordance with QAP-001, and all subsequent in-process entries in accordance with QAP-001. An introduction to the new initial entries shall reference this CAR and serve to explain the out-of-sequence initial entry.

Some Scientific Notebooks are fully compliant with QAP-001; for them remedial action is unnecessary. The Element Manager, with the assistance of QA staff, shall make the determination whether the notebook requires remedial action. Those compliant may be identified by memo to the QA Director. During follow-up surveillance, an accounting of all active notebooks will be made by QA staff, so that remedial action or the Element Manager's determination of compliance are verified.

Proposed Completion Date: November 1, 1996

4) **Corrective Action to Preclude Recurrence:** Retraining on QAP-001 shall be provided to all persons using notebooks. Models of portions of compliant notebooks for code development/analysis as well as laboratory/field investigations shall be provided. These models will establish the level of detail necessary to comply with QAP-001.

Proposed Completion Date: September 20, 1996

E. C. De...
8/27/96

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[55] From: Bruce Mabrito at cnwra-os2 8/15/96 2:30PM (2379 bytes: 40 ln)
To: English Pearcy at CNWRA
cc: Budhi Sagar, Henry Garcia, Robert Brient, Linda Hearon
bcc: Bruce Mabrito, EBass@VEHRES@SwRI03 at SWRI
Subject: Re: Corrective Action Request Responses

----- Message Contents -----

From: English C. Pearcy, Manager GHGC
To: Bruce Mabrito, Director QA
Date: August 15, 1996
Subject: Request for Delay in Response to CAR 96-03

E.C. Pearcy
8/15/96

By this memo, I request a delay in response to CAR 96-03 to Friday August 30, 1996.

TO: CORRECTIVE ACTION RESPONSIBLE EMs:

As noted previously, a Quality Assurance Procedure sets an initial time limit on submission of proposed actions to a corrective action request (CAR). The proposed actions are just that, proposed actions, with a proposed completion date for the remedial action and for the corrective action to preclude recurrence. The proposed completion dates can be days, weeks, or months (hopefully not, but that has occurred before) in the future, depending on the nature of the remedial and corrective actions.

The proposed action response date is tomorrow, Aug. 15th, and that also applies to the CAR on which I am working.

Should you not be able to respond by the COB 8/15/96, please request an extension from me in writing. Each of the EMs have a copy of QAP-010, "Corrective Action," which provides general guidelines for your response. If you need assistance, please call me at x 5149.

Bruce Mabrito 8/13/96

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TO ENGLISH PEARCY / RE CAR 96-03:

Based on the potential work involved in the CAR you are working on and your recent return to the office, I am extending the CAR 96-03 response date to August 30, 1996.

A hard copy of this email document will be and put into the CAR 96-03 folder to provide objective evidence.

Bruce Mabrito

Bruce Mabrito
8/15/96

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Memorandum

To: Bruce Mabrito
 From: English Percy *ECP*
 Date: February 21, 1997
 Subject: Scientific Notebooks

I have completed the assessment of scientific notebooks as requested. The table below indicates the current disposition of the notebooks.

Scientific notebook 162, assigned to W. Murphy/C. Frietas, has not been used. The work Frietas has conducted related to the Yucca Mountain carbon system is only documented in computer input/output files and in papers prepared to report the results of the work. A memo from W. Murphy (attached to this memo) describes the status of the work.

Other notebooks were found to be generally in compliance with QAP-001 or were modified to bring them into general compliance with QAP-001.

NAME	SCIENTIFIC NOTEBOOK #
Turner, David	46, 148, 157A, 177
Winterle, James R.	195*, 197*
Pearcy, English C.	41, 50, 75 80
Wittmeyer, Gordon	76, 77, 113, 166*
Bagtzoglou, A.	65, 67, 68, 69, 145, 146, 171* (Tolley)
Prikryl, James D.	42, 58, 144*, 151, 173*, 198*, 200*
Stothoff, Stuart A.	147, 163E*, 175*
Green, Ronald T.	23, 83, 116, 119 (TEF notebooks reviewed by Asad)
Pickett, David	31*, 121*, 133*, 172*, 126*
Murphy, William M.	37*, 117*, 140*, 162(Frietas), 180*, 192*
Pabalan, Roberto T.	26, 37-1, 61, 81, 82, 185E*

*Active notebooks are indicated by an asterisk.

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Memorandum

To: English C. Pearcy, Peter C. Lichtner, Robert G. Baca
From: William M. Murphy
Date: February 20, 1997

Subject: Status of journal paper on carbon system evolution and scientific notebook documentation

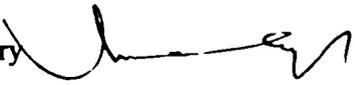
The carbon system paper was completed and submitted to NRC as a deliverable sometime years ago having received normal CNWRA review. It was submitted to the Journal of Contaminant Hydrology in February 1996. It was reviewed and accepted for publication in June 1996. Outside reviewer comments were generally supportive, and addressing reviewer comments would require few changes to the paper. However, model results reported in the paper show some peculiarities that I suspect are due to numerical errors. A plan was devised to resolve this issue and some reviewer comments by performing one additional computation (in two steps) with a finer time and space gridding. This work is still incomplete because it has received lower priority than other work. My recommendation for scientific notebook documentation of the work is to complete the revised modeling, to document the results in revisions to the paper, and then to record the final coding and model results in electronic format. This work will be completed as priorities and time allow.

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

MEMORANDUM

March 6, 1997

TO: Bruce Mabrito
FROM: Asad Chowdhury 
SUBJECT: Scientific Notebooks

I have completed the assessment of scientific notebooks as requested. The table below indicates the current disposition of the notebooks. Some of these notebooks were modified to bring them into general compliance with QAP-001.

Name	Scientific Notebook No.
Hsiung, Simon	17, 18, 63, 64
Ahola, Mikko	179
Mohanty, Sitakanta	106
Rice, George	150*
Green, Ron (TEF Notebooks)	62*, 87*, 104*, 129*
*Ron Green would like to keep these in his office on a temporary basis for use as references.	

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

MEMORANDUM

March 14, 1997

TO: Bruce Mabrito

FROM: Narasi Sridhar *NS*
3/14/97

SUBJECT: Laboratory and electronic scientific notebooks issued to EBS staff

I have examined all the laboratory and hard copies of electronic scientific notebooks as detailed below. Where necessary, the staff has made additional entries such as initial entries or clarification to an existing text to bring these notebooks into compliance with QAP-001. As also noted below, we do not have any record of having received two of the notebooks listed under my name. The Q.A. record also did not indicate these notebooks issued to me. Please correct your records appropriately.

Staff Name	Notebook Number	Disposition
G. Cragnolino	27, 32	Work completed, retaining the notebook till paper is completed.
P. Angell/M. Hill	134, 138, 182	134 will be returned to QA Retaining 138 and 182 for continued use on IR&D project.
D. Dunn	103, 131, 161, 149, 157	Notebooks 157 and 161 will continue to be used. Retaining the other notebooks till copies can be made.
N. Sridhar	9,25,40,45,85,86,109, 124, 125	Notebooks will be returned to QA. Notebooks 124, and 125 were not issued to EBS.
P. Lichtner	095, 102	095 exists as both the standard notebook as well as printouts of electronic notebooks. Will be retained by QA and author. Notebook 102 will be returned to QA.
P. McKeighan	135	Will be returned to QA.

List of Notebooks in the EBS Group

No.	Contents
40	PCT testing of glass simulants 1/17/92 to 5/26/92
95	Hard bound notebook of MULTIFLO/GEM development, 11/16/93 to 12/12/93. Further entries were made in electronic notebooks printed out quarterly with the same number
134	Microbial activities related to both MIC and YM tuff, 3/25/95 to 6/25/96
135	Stress corrosion cracking, fracture mechanics specimen. Most of the record is in charts assembled into binder. Notebook is only initial entry.
102	SCCEX code development. Entry started by Pavitra Ramanujam, summer student. No further entries made.
009	Materials characterization
025	IWPE crevice chemistry, repassivation time tests, repassivation potential tests
027	IWPE stress corrosion cracking, slow strain rate tests U-bend tests
045	IWPE Cyclic Potentiodynamic Polarization tests 304, 316L, 825, C-22, coldworked 825, chromium depleted 825.
085	IWPE crevice chemistry, long-term tests, crevice repassivation tests, galvanic corrosion 316L/creviced 316L, galvanic corrosion alloy 825/creviced alloy 925
103	IWPE Materials stability
131	IR&D In-situ Salt film in pits
149	EBSER Fracture mechanics tests 316L WOL specimens
157	EBSER/ENFE Long-term tests, cyclic potentiodynamic polarization A 516 grade 60
161	IR&D In-situ Salt film in pits, IR&D Wet and dry corrosion
213	Galvanic corrosion calculations

To: Bruce Mabrito
From: Narasi Sridhar
Subject: Scientific notebooks
03-14-97 02:07 PM

Attached is a file that has two tables:

1. Table 1 has the disposition of all the notebooks that were listed under EBS staff. I have reviewed all the notebooks and found them to be in compliance with QAP-001.

2. Table 2 has a description of each of the notebook for your future reference.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 11/54

MEMORANDUM

March 17, 1997

TO: Bruce Mabrito
FROM: Michael P. Miklas, Jr. *MPM*
SUBJECT: Scientific Notebooks Nos. 89, 96, 190

I have completed the technical assessment of the scientific notebooks as requested. The table below indicates the current disposition of the notebooks. The notebook assigned to Pat LaPlante, No. 91, was modified by Pat to bring it into general compliance with QAP-001. This notebook details the changes made by Pat to the original RADTRAN4 code when he was modifying it for use in the SSI Toolbox.

The other two notebooks, Nos. 89 and 96 were used by Ron Janetzke to record the hardware setup and subsequent modifications made to the two Pentium computer systems which were purchased for use in the SSI Toolbox projects. Computer 0 and its accompanying notebook, No. 89, have both been delivered to SSI in Stockholm and are no longer under control of CNWRA. Notebook No. 96 is up to date for Computer 1 which remains at CNWRA.

Name	Scientific Notebook No.
Swedish Radiation Protection Institute Stockholm, Sweden (Computer 0)	89
Ron Janetzke (Computer 1)	96
Patrick Laplante (WO)	91

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Center for Nuclear Waste Regulatory Analyses

MEMORANDUM

March, 19, 1997

To: B. Mabrito
From: R. G. Baca 
Subject: Review of Scientific Notebooks Assigned to TSPA and ARDES KTIs

I have reviewed the scientific notebooks containing information related to the TSPA and ARDES KTIs. The following is a summary of the notebooks reviewed and their status.

A. Nedungadi - #93: Reviewed, signed, and turned in to QA
S. Mohanty - #170E: Reviewed, signed, and returned to author
M. Jarzempa - #130: Reviewed, signed, and turned in to QA
M. Jarzempa - #164: Reviewed, signed, and returned to author
R. Janetzke - #190: Reviewed, signed, and returned to author
P. LaPlante - #178: Reviewed, signed, and returned in author
P. LaPlante - #194: No entries at this time, no review necessary.

This completes my review of the scientific notebooks.

cc:Mail for: larry mckague

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Subject: Completion of scientific notebooks review

From: Larry McKague 4/28/1997 3:10 PM

To: Bruce Mabrito at CNWRA-OS2

All scientific notebooks assigned to the GLGP have been reviewed and found acceptable, including notebook 91 that documents the development of Radtran for SSI project. Except for notebook 91 this work was completed by 4/21/97.

Larry McKague
H. Lawrence McKague
4/28/97

Reviewed Scientific notebooks

Number	Type	Responsible	Date reviewed	Holder	Name	
33		David Ferrill	4/19/97	Alan Morris	Morris	To be archived
34		John Stamatakos	4/18/97	Raymond Donlick	Donlick	To be archived with additional bound material
51		David Ferrill	4/21/97	Alan Morris	Morris	To be archived
54		David Ferrill	4/18/97	Alan Morris	Morris	To be archived
56	E	Brit Hill	Archived 1/3/97		Hill	
59		John Stamatakos	4/18/97		Stamatakos	
72		Chuck Connor	Archived		Connor	
73		Chuck Connor	Archived		Connor	
79		Chuck Connor	Archived		Connor	
88	E	Brit Hill	4/14/97		Hill	
90		Brit Hill	4/16/97	Steve Linton	Linton	Reviewed by B. Mabrito 4/16/97
91		Mike Miklas	4/28/97		Miklas	SSI Notebook (P. LaPlant) Archived 4/28/97
97		Brit Hill	4/16/97	Steve Linton	Linton	Reviewed by B. Mabrito 4/16/97
99		John Stamatakos	4/17/97		Stamatakos	
100		David Ferrill	3/17/97		Ferrill	
101		David Ferrill	1/14/97		Ferrill	
113		Brent Henderson	Archived		Henderson	
115	E	Chuck Connor	4/17/97		Connor	
128		David Ferrill	3/4/97		Ferrill	Ann Blyth
136		Larry McKague	3/28/97	Robert Terhune	Terhune	Reviewed by B. Brient 1995(?)
136	E	Larry McKague	3/28/97	Robert Terhune	Terhune	
137		Larry McKague	3/28/97	Robert Terhune	Terhune	
137	E	Larry McKague	3/28/97	Robert Terhune	Terhune	
141		David Ferrill	2/6/97		Ferrill	Brett Rahe
142		David Ferrill	3/17/97		Ferrill	
154		David Ferrill	4/18/97	Alan Morris	Ferrill	To be archived
155		Larry McKague	4/18/97	Larry McKague	Stamatakos	
156		John Stamatakos	See Comment		Stamatakos	This notebook has not been placed in use
181		David Ferrill	4/16/97	William Dunne	Dunne	Reviewed by B. Mabrito 4/16/97
189		David Ferrill	3/11/97	Darrel Sims	Simms	

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 15/54

MEMORANDUM

September 20, 1996

TO: QA Records Corrective Action Request 96-03 File
FROM: Bruce Mabrito, Director of Quality Assurance 
SUBJECT: Status of Corrective Actions on CAR 96-03 as of 9/20/96
REFERENCE: CAR 96-03, From Annual CNWRA QA Audit

This memorandum to the CAR 96-03 file is to document progress to date to complete corrective actions.

Item 4 on the Corrective Action Request for 96-03 stated that the corrective action to preclude recurrence was "retraining on QAP-001 shall be provided to all persons using (scientific) notebooks. Models of portions of compliant notebooks for code development/analysis as well as laboratory/field investigations shall be provided. These models will establish the level of detail necessary to comply with QAP-001." The proposed completion date for this activity was set for September 20, 1996.

During the past two weeks, conversations have taken place on the best approach to provided effective retraining in this area and several "model" scientific notebooks have been identified, however the actions are not yet complete by any means. The proposed completion date of September 20, 1996 was too ambitious with the other corrective actions that are also ongoing since the audit.

The proposed completion date for corrective actions to preclude recurrence regarding CAR 96-03 is upon us and, based on the progress to date and the need to resolve other issues related to CAR 96-03, I am extending the proposed completion date for the corrective action to preclude recurrent to October 18, 1996.

If there are any questions regarding this change, please contact me at ext. 5149.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 11/54

MEMORANDUM

October 18, 1996

TO: QA Records Corrective Action Request 96-03 File

FROM: Bruce Mabrito, Director of Quality Assurance *Bruce Mabrito*

SUBJECT: Status of Corrective Actions on CAR 96-03 as of 10/18/96

REFERENCE: CAR 96-03, From Annual CNWRA QA Audit

This memorandum to the CAR 96-03 file is to document progress to date to complete corrective actions.

During the regular QA surveillances, scientific notebooks have been checked as a normal part of the surveillance activity. Additionally, discussions have been held with some of the CNWRA Element Managers to ascertain the best method to ensure that CNWRA scientific notebooks have sufficient initial entry and in-process entries to describe the "planning, objectives, methods, or results" (quote from the CAR) such that there is "a high confidence that another qualified individual might understand and/or repeat the activity." To date, the CNWRA QA group has not received feedback from the Element Managers that they have made the determination whether a scientific notebook requires remedial action.

Since the audit, numerous CNWRA staff have been visited by the QA staff and their scientific notebooks have been checked and training has taken place, however in most cases this training has not been documented.

The proposed completion date for corrective actions to preclude recurrence regarding CAR 96-03 is not yet complete because of other pressing business (including the budget reductions, Operations Plan development, KTI changes, and related activities). Based on the progress to date, I am extending the proposed completion date for the corrective action to preclude recurrence ("retraining on QAP-001 shall be provided to all persons using notebooks") to November 22, 1996.

If there are any questions regarding this change, please contact me at ext. 5149.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 17/54

MEMORANDUM

November 22, 1996

TO: QA Records Corrective Action Request 96-03 File

FROM: Bruce Mabrito, Director of Quality Assurance 

SUBJECT: Status of Corrective Actions on CAR 96-03 as of 11/22/96

REFERENCE: CAR 96-03, From Annual CNWRA QA Audit

This memorandum to the CAR 96-03 file is to document progress to date to complete corrective actions.

Scientific notebooks continue to be checked during scheduled QA surveillances. Discussions continue to be held with CNWRA Element Managers to ensure they are aware of the need to have scientific notebooks in their Element with sufficient initial and in-process entries to describe the planning, objectives, methods, or results so that there is high confidence that another qualified individual might understand and/or repeat the activity.

Additionally, during the "all hands" quarterly CNWRA staff meeting November 20, 1996, training took place with all persons present regarding initial and in-process entries to scientific notebooks (see attachment "Scientific Notebook 'Hints and Tips' Sheet"). However, the full proposed remedial action has not been completed. It should be noted that there will be a "turn in" of a large number of Research Project scientific notebooks immediately after the start of the calendar year. Many of the scientific notebooks will be submitted through the Element Managers to the QA Records and that will be an opportunity to complete the corrective actions in this CAR.

Based on the above, the completion date for corrective actions regarding CAR 96-03 needs to be extended. I am extending the completion date for the corrective actions to preclude recurrent to January 31, 1997.

If there are any questions regarding this change, please contact me at ext. 5149.

18/54

CNWRA QUARTERLY STAFF MEETING
November 20, 1996
3:00 – 5:00 PM
Bldg 189 Shared Conference Room

AGENDA

- 1) **Staffing Outlook** **W. Patrick**
- 2) **Quick Items** **W. Patrick**
 - Evaluation by the Center Review Group (CRG)
 - Plans for Contract Renewal
 - Feedback from Annual Review Meeting
- 3) **Business Development Activities** **B. Sagar**
- 4) **Selected Items from CNWRA Management Meeting at Austin** **E. Pearcy**
- 5) **Standardization of CNWRA-approved Software** **H. Garcia**
 - Installation
 - Removal of Unlicensed Software
- 6) **Scientific Notebooks** **B. Mabrito**
- 7) **CNWRA Christmas Dinner/Party** **All**
- 8) **Any Other Items**
- 9) **Next Meeting: Wednesday, February 21, 1997, 10–12 Noon**
(Shared Conference Room B189)

cc: **WTSO**

H:\BUDHI\QTRMTG.COR\AGEN1196.QM

SCIENTIFIC NOTEBOOK "HINTS AND TIPS" SHEET (Highlights from QAP-001)

INITIAL ENTRIES:

- On Electronic Scientific Notebooks (SNs), please show SN number.
- List title of experiment (including project number).
- List names of all individuals performing the activity.
- Describe the objectives and approach (can be from the OPS Plan).
- List and identify special personnel training or qualification requirements.

NOTE: Since electronic SNs often are ongoing (volume-after-volume every 3 months), please have a title page for each printing indicating the initial entries and the date printed. Each page should be sequentially numbered (i.e., 1, 2, 3, etc.) as indicated in QAP-001 Section 3.6.4.

COMPUTER/SOFTWARE ANALYSES:

- Describe the hypothesis to be evaluated or give list of objectives.
- Summarize the technical approach to be used.
- Briefly describe the mathematical theory, assumptions, boundary conditions, solution algorithm(s), computer software, reference documents, etc.
- Include the configuration management status of the software, computer platform used, directory and file names where codes are located.
- Refer to aspects affecting computational reliability and the approach to be used to evaluate grid and time step refinements and comparisons with other approaches.

IN-PROCESS ENTRIES:

- SN entries shall be made daily, or as appropriate, throughout the work activities and shall be sufficiently detailed so that another qualified individual can understand and/or repeat the activity.
- Describe what you have done in a step-by-step fashion (referencing procedures, standards, guidelines in other documents, if that's what you followed).
- Include information such as key data sets, code test results, analysis results, calibration information, description of problems encountered, alternative actions considered, actions taken in response to problems.
- Document significant changes or variances from the original plan.
- Concisely describe principal computational results and interim conclusions drawn; significant computational results shall be saved and incorporated by reference (keeping a copy of the electronic input and output files with the SN is advised...when a product is completed, the Technical Director has requested input and output data be filed with the document reviews in the QA Records).
- Give results/final interpretations/conclusions drawn for each step of the process.

PROTOCOL:

Each initial entry and each in-process entry must be signed and dated by the authorized individual making the entry. Use permanent ink. Make corrections with single line and initial. Electronic SNs shall be printed out quarterly, as in March, June, September, and December. If no work was accomplished on the task during the quarter, a statement should be sent to CNWRA QA for the permanent records.

Re: Scientific Notebook Reviews by [redacted] is

20/5/4

To: Bruce Mabrito
From: Robert Baca
Subject: Re: Scientific Notebook Reviews by EMs
12-12-96 04:13 PM

From our discussion in the Management Staff meeting Monday, these two pieces of information.

First, English and Sridhar have responded to my request to estimate how long it will take them to completely review the scientific notebooks in their areas. A tentative date is now the 15th of January. Other Element Managers should let me know if this is an acceptable date, based on their total number of notebooks and availability of staff.

Second, if the Element Manager review determines that a scientific notebook has sufficient technical detail in an acceptable format, a statement such as the following should be entered in the scientific notebook:

"I have reviewed this scientific notebook and find it in general compliance with QAP-001 and there is sufficient technical information so that another qualified individual could repeat the activity.
(signed) _____ Element (date)"

Bruce

=====
Bruce:

The above date is OKay with me.

Cheers, Bob.
=====

2/5/97

To: Bruce Mabrito
From: Narasi Sridhar
Subject: Re: CAR 96-03 Actions - Scientific Notebook Reviews
02-24-97 07:25 AM

NOTE: This message is specifically addressed to CNWRA Element Managers who are working on this corrective action.

Late Friday I received a memo from English Percy which described his completion of his assessment of scientific notebooks as described in Corrective Action Request 96-03. I have provided each of the EMs a copy of the memo, which is more comprehensive than I expected to receive, but most certainly welcome.

At this time I am requesting a similar memorandum from each of the EMs who have reviewed CNWRA scientific notebooks to determine whether they are "technically sufficient" to meet the test that "another qualified individual might understand and/or repeat the activity."

Thanks for your efforts to date in this long corrective action and please call me if I can assist you to complete this work.

Bruce

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Bruce:

I am working through them. I had to put those aside to complete the Hanford familiarization report. I hope to complete the reviews by the end of this week. Sorry for the delay. Thanks

Sridhar

22/54

TO Mail List:#DIRS-MGRS
To: Larry McKague at CNWRA
To: English Percy at CNWRA
CC: Linda Hearon
BCC: Bonnie Caudle
BCC: Bruce Mabrito
BCC: Robert Brient
From: Bruce Mabrito
Subject: Corrective Action Request 96-03 - Status
01-15-97 09:43 PM

Element Managers:

Several CNWRA Element Managers have discussed with me their progress in checking the Scientific Notebooks in their respective Elements. Progress has been substantial, and from the comments I have received, improvement in the notebooks have been realized through this process.

In some cases, EMs are returning notebooks to the PI or notebook author for additions, corrections, or modifications so that another qualified individual will understand and be capable of repeating the activity. Based on the discussions I have had, it would appear that the remedial actions are about 75-percent complete at this time.

Considering the progress to date and that a few EMs have had to call in notebooks from other locations to review them, I have been asked by several EMs to extend the date to complete this remedial action. By this email message, I am extending the completion date to February 21, 1997.


Bruce Mabrito

cc: W. Patrick
B. Sagar
CAR 96-03 Folder

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES ^{23/24}

MEMORANDUM

February 21, 1997

TO: QA Records Corrective Action Request 96-03 File
FROM: Bruce Mabrito, Director of Quality Assurance 
SUBJECT: Status of Corrective Actions on CAR 96-03 as of 2/21/97
REFERENCE: CAR 96-03, Annual CNWRA QA Audit

This memorandum to the CAR 96-03 file is to document progress to date to complete corrective actions.

Item 4 on the Corrective Action Request for 96-03 stated that the corrective action to preclude recurrence was "retraining on QAP-001 shall be provided to all persons using (scientific) notebooks. Models of portions of compliant notebooks for code development/analysis as well as laboratory/field investigations shall be provided. These models will establish the level of detail necessary to comply with QAP-001." The last proposed completion date for this activity was set for February 21, 1997.

This training has been provided to all but the GLGP Element over the past months. Due to travel by the GLGP and NRC staff, no GLGP Element meeting has taken place and therefore no such training has been provided. I have been assured that the next GLGP Element meeting will be within three weeks, at which time the QA QAP-001 training will be provided regarding this topic and other related QA topics.

Additionally, all CNWRA Element Managers have been provided a listing of scientific notebooks for which they have "technical responsibility" and they have been reviewing such scientific notebooks to ensure that there is "high confidence that another qualified individual might understand and/or repeat the activity," to quote from CAR 96-03. That work is over 90-percent complete and the GHGC Element Manager has provided his notification of the scientific notebooks he has reviewed. In some cases, EMs have sent back scientific notebooks to the PI so that more technical detail can be provided. At this time, all such reviews are yet completed, but definite progress has been reported to CNWRA QA staff and has been verified by QA staff. Based on this progress, it appears appropriate to extend the proposed completion date to March 21, 1997.

If there are any questions regarding this change, please contact me at ext. 5149.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES ^{24/54}

MEMORANDUM

March 21, 1997

TO: QA Records Corrective Action Request 96-03 File

FROM: Bruce Mabrito, Director of Quality Assurance 

SUBJECT: Status of Corrective Actions on CAR 96-03 as of 3/21/97

REFERENCE: CAR 96-03, Annual CNWRA QA Audit

This memorandum to the CAR 96-03 file is to document progress to date to complete corrective actions.

Item 4 on the Corrective Action Request for 96-03 stated that the corrective action to preclude recurrence was "retraining on QAP-001 shall be provided to all persons using (scientific) notebooks." Such retraining for CNWRA staff was completed 3/13/97 with the last presentation to the GLGP Element.

All CNWRA Element Managers were provided a listing of scientific notebooks for which they have "technical responsibility" and they have been reviewing such scientific notebooks to ensure that there is "high confidence that another qualified individual might understand and/or repeat the activity," according to CAR 96-03. That work by the CNWRA Element Managers is over 95-percent complete and all but one Element Manager has provided the objective evidence of the EM review by the date of this memorandum. In one case, the EM has checked over half of the scientific notebooks assigned in his area, but has requested a completion date extension to check the remainder of scientific notebooks, including several notebooks being utilized by a consultant located in another state. Progress of the corrective actions identified in CAR 96-03 is nearly finished, however the GLGP EM said that because of NRC-mandated travel it will take him until April 11, 1997 to ensure all work is completed. Considering the steady progress of the corrective and remedial actions and the objective evidence provided by the EMs, it appears appropriate to extend the proposed completion date to April 11, 1997.

If there are any questions regarding this change, please contact me at ext. 5149.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 25/54

MEMORANDUM

April 28, 1997

TO: QA Records Corrective Action Request 96-03 File

FROM: Bruce Mabrito, Director of Quality Assurance



SUBJECT: Closure of CAR 96-03

REFERENCE: CAR 96-03 from Annual CNWRA QA Audit

This memorandum to Corrective Action Request 96-03 file is to document closure of this CAR.

The final required actions to close out CAR 96-03 have now taken place.

The Element Managers have completed their reviews of CNWRA scientific notebooks and have documented such reviews by memoranda to QA. In some cases, CNWRA scientific notebooks were submitted to QA Records following the review rather than being returned to the Principal Investigator or individual maintaining the scientific notebook because they were determined to be complete by the EM.

Because of the delay in closing this and other CARs, another CAR (97-01) was written because of the delays that seemed to be system wide at the CNWRA.

2/15/97

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES MEETING ATTENDANCE

SUBJECT OF MEETING *QA Training for GLGP Element*

DATE: *3/13/97* LOCATION: *CNWRRA Conference Rm A137*

PERSON	ORGANIZATION	TITLE/FUNCTION	TELEPHONE NUMBER
<i>Annette Manduyano</i>	<i>CNWRRA</i>	<i>Secretary</i>	<i>5472</i>
<i>R. MARTIN</i>	<i>SURI</i>	<i>Staff</i>	<i>5541</i>
<i>M. W. Conway</i>	<i>CNWRRA</i>	<i>Staff</i>	<i>6829</i>
<i>C. Conner</i>	<i>"</i>	<i>"</i>	<i>6649</i>
<i>C. McELKAGUE</i>	<i>"</i>	<i>EM GLGP</i>	<i>5183</i>
<i>Mike Miklas, Jr.</i>	<i>CNWRRA</i>	<i>Sr. Res. Scientist</i>	<i>522-5207</i>
<i>John Stamatikos</i>	<i>"</i>	<i>Pin Question</i>	<i>522 5247</i>
<i>Bertina Hill</i>	<i>"</i>	<i>Res Sci</i>	<i>56087</i>
<i>DAN FERRELL</i>	<i>CNWRRA</i>	<i>Sr. Res. Sci.</i>	<i>6082</i>

*Subject TRAINING Took place for approximately
one hour and covered subjects: QAP-014,
QAP-001, subcontracts, CNWRRA Philosophy
of integration of disciplines, subcontracts,
scientific notebooks, and related subjects.*

*Lots of feedback obtained from GLGP staff
on QAP-014, Rev 1, Chg 0. Scientific Notebook
updates and maintenance was stressed.*

*John Miklas
3/13/97*

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES MEETING ATTENDANCE

SUBJECT OF MEETING *QA TRAINING FOR EBS ELEMENT*

DATE: *1/24/97* LOCATION: *Conference Room A132*

PERSON	ORGANIZATION	TITLE/FUNCTION	TELEPHONE NUMBER
<i>GUSTAVO CRAGNOLINO</i>	<i>CNWRP</i>	<i>Staff Sci</i>	<i>X 5539</i>
<i>N. Friedrich</i>	<i>"</i>	<i>EMERSON</i>	<i>5338</i>
<i>P. Lichten</i>	<i>"</i>	<i>Prin Sci</i>	<i>6084</i>
<i>Peter Angell</i>	<i>"</i>	<i>visiting Sci</i>	<i>5797</i>
<i>DARRELL DUNN</i>	<i>"</i>	<i>RES ENGR</i>	<i>6090</i>
<i>Bernie L Garcia</i>	<i>"</i>	<i>Secretary</i>	<i>5217</i>

Subject Training Took place for an hour and dealt with QAP-014, QAP-001, subcontracts, CNWRP philosophy of discipline integration and related subjects. Scientific notebook upkeep and maintenance was stressed.

Bernie Garcia 1/24/97

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

MEETING ATTENDANCE

29/97

SUBJECT OF MEETING: *Quality Assurance Training GNGC Element*

DATE: *1/2/97* LOCATION: *A237*

PERSON	ORGANIZATION	TITLE/FUNCTION	TELEPHONE NUMBER
<i>S. Stothoff</i>	<i>CNWRA</i>	<i>RF3 Sci</i>	<i>x 5208</i>
<i>Gordon Wittmayer</i>	<i>CNWRA</i>	<i>Sr. Res. Sci.</i>	<i>x 5082</i>
<i>David Pickett</i>	<i>CNWRA</i>	<i>Res Sci</i>	<i>5582</i>
<i>Jim Pickett</i>	<i>CNWRA</i>	<i>Res Sci</i>	<i>5667</i>
<i>Ron Green</i>	<i>CNWRA</i>	<i>Sr. Res Sci</i>	<i>5305</i>
<i>Roberto Malanda</i>	<i>CNWRA</i>	<i>Sr. Res Sci</i>	<i>5304</i>
<i>E. Perry</i>	<i>CNWRA</i>	<i>Eng. GNGC</i>	<i>5540</i>
<i>Jim Witterle</i>	<i>CNWRA</i>	<i>scientist</i>	<i>5249</i>
<i>William Murphy</i>	<i>CNWRA</i>	<i>Principal Scientist</i>	<i>5263</i>
<i>David R. Jones (42)</i>	<i>CNWRA</i>	<i>Sr. Res. Scientist</i>	<i>x2139</i>
<p><i>Subject Training took place for approximately 1 hour and dealt with QAP-14, QAP-001, subcontractors, CNWRA philosophy of integration of disciplines, and related subjects. Scientific Notebook revision was discussed and all of QAP-014, "Documentation and Verification of Scientific and Engineering Calculations, Rev 1, Chg 0, was taught. Scientific Notebook maintenance was stressed.</i></p> <p style="text-align: right;"><i>Roberto Malanda</i> <i>1/2/97</i></p>			

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

MEETING ATTENDANCE

30/84

SUBJECT OF MEETING *Quality Assurance Training - RDCO Element*

DATE: *12/9/96*

LOCATION: *CNWRA Conf. Rm A137-616 189*

PERSON	ORGANIZATION	TITLE/FUNCTION	TELEPHONE NUMBER
<i>MIKKO AHOLA</i>	<i>CNWRA</i>	<i>Sr Res Eng</i>	<i>x5799</i>
<i>Asad Chowdhury</i>	<i>CNWRA</i>	<i>Manager - RDCO</i>	<i>x5151</i>
<i>Rui Chen</i>	<i>CNWRA</i>	<i>Res Eng</i>	<i>x5152</i>
<i>YOLANDA LOZANO</i>	<i>CNWRA</i>	<i>Secretary</i>	<i>5384</i>
<i>Goodluck Ojo</i>	<i>CNWRA</i>	<i>Sr Res Eng</i>	<i>6641</i>
<i>Simon Hsiung</i>	<i>CNWRA</i>	<i>Pri. Eng</i>	<i>5209</i>
<i>Amitava Ghosh</i>	<i>CNWRA</i>	<i>Senior Research Engineer</i>	<i>3314</i>
<p><i>Training took place for approximately</i></p> <p><i>2 hours and dealt with QAP-001, subcontracts,</i></p> <p><i>CNWRA philosophy of integration of disciplines,</i></p> <p><i>and related subjects. Scientific notebooks</i></p> <p><i>was discussed, including the EPA Review</i></p> <p><i>of such notebooks in response to a 1996</i></p> <p><i>Audit contractor's action request. Last, QAP-001</i></p> <p><i>"Documentation and Verification of Scientific</i></p> <p><i>and Engineering Calculations," Revision 1</i></p> <p><i>Change 0 was taught. Scientific notebook maint-</i></p> <p><i>ance was stressed.</i></p> <p style="text-align: right;"><i>Sam W. ...</i></p> <p style="text-align: center;"><i>12/9/96</i></p>			

UNCONTROLLED

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES	Proc. QAP-014 Revision <u>1</u> Chg <u>0</u> Page <u>1</u> of <u>4</u>
QUALITY ASSURANCE PROCEDURE	

Title

QAP-014 DOCUMENTATION AND VERIFICATION
OF SCIENTIFIC AND ENGINEERING CALCULATIONS

EFFECTIVITY AND APPROVAL

Revision 1 of this procedure became effective on 10/14/96 . This procedure consists of the pages and changes listed below.

<u>Page No.</u>	<u>Change</u>	<u>Date Effective</u>
All	0	10/14/96

UNCONTROLLED
Bruce Mabrito

Supersedes Procedure No. QAP-014, Rev. 0, Chg 0 dated 05/31/91.

Approvals

Written By <i>Robert Brient</i> Robert Brient	Date 10/14/96	Concurrence Review <i>Budhi Sagar</i> Budhi Sagar	Date 10/14/96
Quality Assurance <i>Bruce Mabrito</i> Bruce Mabrito	Date 10/14/96	Cognizant Director <i>H. Garcia</i> Henry Garcia	Date 10/14/96

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**CENTER FOR NUCLEAR WASTE
REGULATORY ANALYSES**

QUALITY ASSURANCE PROCEDURE

Proc. QAP-014

Revision 1 Chg 0

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**QAP-014 DOCUMENTATION AND VERIFICATION
OF SCIENTIFIC AND ENGINEERING CALCULATIONS**

1. **PURPOSE**

The purpose of this procedure is to specify the methods for documenting and verifying scientific and engineering calculations. This procedure applies to calculations performed by hand, hand calculator, and by computer software.

2. **RESPONSIBILITIES**

2.1 The investigator is responsible for documenting calculations in an appropriate Scientific Notebook as specified in this procedure.

2.2 Technical reviewers are responsible for verifying samples of calculations as specified in this procedure.

3. **PROCEDURE**

3.1 **Documentation of Calculations**

Calculations shall be documented in appropriate Scientific Notebooks sufficiently so that the calculation can be duplicated. Data inputs, the calculational methods, and data outputs shall be documented as follows:

3.1.1 Data inputs, including those used in (i) simple calculations (i.e., those that can be easily duplicated by a hand calculator); (ii) complex numerical analysis by uncontrolled software; and (iii) complex numerical analysis by software controlled under TOP-18, shall be documented by direct recording of the data or by reference. Any reference should identify the source of the data, such as (i) another calculation; (ii) a report; (iii) an engineering handbook, periodic table, or other accepted source; or (iv) a laboratory or field notebook.

3.1.2 Computational methods shall be documented according to the method of calculation.

(i) **Simple Calculations** — The algorithm used or reference to a standard method shall be recorded in the scientific notebook unless obvious to a qualified technical reviewer.

**CENTER FOR NUCLEAR WASTE
REGULATORY ANALYSES**

QUALITY ASSURANCE PROCEDURE

Proc. QAP-0014

Revision 1 Chg 0

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(ii) Uncontrolled Software — Software not under TOP-018 control shall be identified by name and version in the scientific notebook and in reports presenting the results of the calculation. To preserve the exact configuration of the software used in the calculation, a copy of the software shall be archived and submitted in the review package of the associated reports. The Scientific Notebook shall include a justification for the use of the software for the specific application. In addition, one or more test cases, appropriate for the specific application of the software, shall be run to demonstrate proper operation of the software, and shall be documented in the Scientific Notebook.

(iii) Controlled Software — Software which has been controlled and released in accordance with TOP-018 shall be identified by name and version number in the Scientific Notebook and in associated reports. Additionally, justification for the use of the software for the specific application shall be documented in the Scientific Notebook.

3.1.3 Output data for calculations shall be documented in the appropriate Scientific Notebook. If the output data consist of large files, the files may be copied to a disk and attached to the Scientific Notebook or the Scientific Notebook may reference a file location. Electronic output files should identify the software name and version and date of the calculation.

3.2 Verification of Calculations

In accordance with QAP-002, the Element Manager shall check the technical review criterion associated with QAP-014 for technical reports which involve scientific or engineering calculations. The designated Technical Reviewer shall identify data within the report that were or appear to have been derived through calculation (i.e., data not directly referenced to another source), and shall sample at least 10 percent of the data for verification or as required by contract. The Technical Reviewer shall obtain the appropriate Scientific Notebooks from the investigator(s), and with the assistance of the investigator, locate the sampled calculations.

3.2.1 The Technical Reviewer shall verify that the input data have been documented as required in paragraph 3.1.1.

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**CENTER FOR NUCLEAR WASTE
REGULATORY ANALYSES**

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QUALITY ASSURANCE PROCEDURE

- 3.2.2 The Technical Reviewer shall verify that the calculational methods have been documented as required in paragraph 3.1.2., sections (i), (ii), or (iii) as appropriate.
- 3.2.3 The Technical Reviewer shall verify that the output data have been documented, and that the calculations have been correctly performed, as follows:
 - (i) Simple Calculations — Simple calculations (originally performed by hand, hand calculator, spread sheet, or statistical software) within the sample shall be verified by duplicate calculations.
 - (ii) Uncontrolled Software — Calculations performed by uncontrolled software within the sample shall be verified by checking that the input data have been correctly transferred (values, units, etc.) to the input data deck. The output data (including any post-processing of data) shall be evaluated for reasonableness considering the input data and calculation performed.
 - (iii) Controlled Software — Calculations performed by controlled software within the sample shall be verified by checking that the input data have been correctly transferred (values, units, etc.) to the input data deck. The output data (including any post-processing of data) shall be evaluated for reasonableness considering the input data and calculation performed.
- 3.2.4 Verifications shall be documented on the report comment resolution sheets (CNWRA Form TOP-3), identifying the location of the calculation by Scientific Notebook number and page. Any duplicate calculations [see paragraph 3.2.3(i)] shall be documented on or attached to the comment resolution sheet.
- 3.2.5 Any discrepancies between the calculation documentation and those required by this procedure shall be recorded as technical review comments requiring resolution. Resolution shall be by amending the calculation documentation so that the requirements of this procedure are met.

4. RECORDS

No records are generated as a result of this procedure. Technical review comment resolution sheets shall be retained as QA records in accordance with QAP-002.

CNWRA SCIENTIFIC NOTEBOOK

- **Follow QAP-001**
- **Follow "Hints & Tips" Issued at Quarterly Staff Meeting**
- **Submit Electronic Scientific Notebooks Promptly When Asked**
- **Keep Track of Your S/N – You Are Responsible For It**
- **Prepare to Submit Your Notebook to Your EM for Review ASAP (Correction Action Request 96-03)**

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PREPARATIONS OF SUBCONTRACTOR CONTRACTS

- **Administrative Procedure-005, "Subcontract Submission and Approval" and Quality Assurance Procedure-016, "Procurement Control" Tells How**
 - **Freedom From Any Organizational COI**
 - **Documented Competence in Technical Areas**
 - **Demonstrated Record of Completing Work in a Timely & Cost-Effective Manner**
 - **Director of QA Responsible for Providing Quality Requirements**
 - **Element Managers/Cognizant Directors Responsible for Approving Purchase Requisitions**

3/6/54

PREPARATIONS OF SUBCONTRACTOR CONTRACTS (cont'd)

- **Purchase Requisition Shall Identify:**
 - **Scope of Work, Services Required**
 - **Applicable Codes, Regulations, Specifications, Standards or Technical Requirements**
 - **Certification Requirements**
 - **Certification of Special Processes**
 - **Requirements for Special Documentation**
 - **Quality Requirements**

PREPARATIONS OF SUBCONTRACTOR CONTRACTS (cont'd)

- **Supplier Qualification**
 - **Documented History of Providing Products Meeting Technical & Quality Capability**
 - **Evaluation of Supplier Technical & Quality Capability**
 - **Qualification in Accordance with SwRI NQAPM Qualified Vendors List**

- **Acceptance of Services**

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"OTHER THINGS"

- **CNWRA Philosophy**
 - **Vision Statement**
 - **CNWRA Indoctrination Packet**

**Integration — We Inform Each Other of What We're Doing.
Examples**

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SCIENTIFIC NOTEBOOK "HINTS AND TIPS" SHEET (Highlights from QAP-001)

INITIAL ENTRIES:

- On Electronic Scientific Notebooks (SNs), please show SN number.
- List title of experiment (including project number).
- List names of all individuals performing the activity.
- Describe the objectives and approach (can be from the OPS Plan).
- List and identify special personnel training or qualification requirements.

NOTE: Since electronic SNs often are ongoing (volume-after-volume every 3 months), please have a title page for each printing indicating the initial entries and the date printed. Each page should be sequentially numbered (i.e., 1, 2, 3, etc.) as indicated in QAP-001 Section 3.6.4.

COMPUTER/SOFTWARE ANALYSES:

- Describe the hypothesis to be evaluated or give list of objectives.
- Summarize the technical approach to be used.
- Briefly describe the mathematical theory, assumptions, boundary conditions, solution algorithm(s), computer software, reference documents, etc.
- Include the configuration management status of the software, computer platform used, directory and file names where codes are located.
- Refer to aspects affecting computational reliability and the approach to be used to evaluate grid and time step refinements and comparisons with other approaches.

IN-PROCESS ENTRIES:

- SN entries shall be made daily, or as appropriate, throughout the work activities and shall be sufficiently detailed so that another qualified individual can understand and/or repeat the activity.
- Describe what you have done in a step-by-step fashion (referencing procedures, standards, guidelines in other documents, if that's what you followed).
- Include information such as key data sets, code test results, analysis results, calibration information, description of problems encountered, alternative actions considered, actions taken in response to problems.
- Document significant changes or variances from the original plan.
- Concisely describe principal computational results and interim conclusions drawn; significant computational results shall be saved and incorporated by reference (keeping a copy of the electronic input and output files with the SN is advised...when a product is completed, the Technical Director has requested input and output data be filed with the document reviews in the QA Records).
- Give results/final interpretations/conclusions drawn for each step of the process.

PROTOCOL:

Each initial entry and each in-process entry must be signed and dated by the authorized individual making the entry. Use permanent ink. Make corrections with single line and initial. Electronic SNs shall be printed out quarterly, as in March, June, September, and December. If no work was accomplished on the task during the quarter, a statement should be sent to CNWRA QA for the permanent records.

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To: Budhi Sagar
To: Robert Baca
To: English Pearcy at CNWRA
CC: Henry Garcia
CC: Wesley Patrick
BCC: Bruce Mabrito
BCC: Linda Hearon
BCC: rbrient@swri.edu at Internet
From: Bruce Mabrito
Subject: Overdue Condition on Corrective Action Requests 96-01/96-03
04-11-97 07:51 PM

April 11, 1997 was the proposed completion date for two Corrective Action Requests, 96-01 regarding TOP-018 compliance, and 96-03, regarding scientific notebook entries. As of this date, the full corrective actions have not been accomplished.

Both CARs have been open since the 1996 QA Audit which was completed 7/26/96. There have been numerous extensions provided and, although considerable progress has been made over the months in both the areas, the full Corrective Action process is not yet complete. I have signed a quarterly quality trend analysis which identifies that our corrective action process has not received attention and priority to correct the conditions. A Corrective Action Request 97-01 has been provided to B. Sagar on the subject of corrective actions not appearing to have been given the priority needed for prompt correction. The CAR requires addressing (i) the extent of the condition, (ii) root cause, (iii) remedial action, and (iv) corrective action to preclude recurrence.

A copy of this e-mail message will be put in the respective CAR folders. Bruce Mabrito

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Printed: April 30, 1997

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS:

PCZ

SCIENTIFIC NOTEBOOK

by

Peter C. Lichtner

**Southwest Research Institute
Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas**

SAMPLE

ELECTRONIC

For Period: First Quarter

SCIENTIFIC

January 1, 1997 — March 30, 1997

NOTEBOOK

Printed April 30, 1997

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Printed: April 30, 1997

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS: PCZ

INITIAL ENTRIES

Scientific NoteBook: # 095

Issued to: P. C. Lichtner

Issue Date: Tuesday, November 16, 1993

Computerized Initials: PCZ

By agreement with the CNWRA QA this NoteBook is to be printed at approximate quarterly intervals. This computerized Scientific NoteBook is intended to address the criteria of CNWRA QAP-001.

Table 1: Computing Equipment

Machine Name	Type	OS	Location
gravenstein.cnwra.swri.edu	Pentium Workstation	NEXTSTEP	desk Rm A-126
	133 Mhz	Version 3.3	Bldg. 189
	64 MB RAM		
skippy.cnwra.swri.edu	Sun SPARC 20	SUNOS 4.1.2	network
	96 MB RAM		

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Printed: April 30, 1997

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS:

PC

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1 REFERENCES 27

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PCZ

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1 Increase in chloride concentration as water is evaporated from a container initially filled with 1 kg of water as described by Eqn.(1). To convert to molality note that 1000 mg/liter chloride is equivalent to 0.0282 molal. 2

2 Enrichment factor for chloride at 100 years plotted as a function of depth computed using MULTIFLO with a residual saturation of 0.08 (solid curve) and 0.01 (dashed curve) compared with the simple evaporation model (dotted curve $s_l^r = 0.08$, dash-dotted curve $s_l^r = 0.01$) 13

3 Enrichment factor for chloride at the repository horizon plotted as a function of time computed using MULTIFLO with residual saturations of 0.08 (solid curve) and 0.01 (dashed curve) compared with the simple evaporation model (dotted curve $s_l^r = 0.08$, dash-dotted curve $s_l^r = 0.01$). 14

4 Log permeability enhancement factor plotted as a function of the exponent n in Eqn.(12) for the alteration of cristobalite to quartz. The solid line is for an initial cristobalite volume fraction of 0.14, and the dashed line 0.39 used by Johnson and Glassley. 16

5 Volume fractions for cristobalite (dotted curve) and quartz (dashed curve) depicted as a function of depth for an elapsed time of 1000 years. Also shown is the porosity (solid curve). Calculations were performed using MULTIFLO based on the repository-scale model. 17

6 Repository-scale model. 19

7 Temperature at the repository horizon plotted as a function of time. 20

8 The liquid saturation at the repository horizon plotted as a function of time. 20

9 The pH plotted as a function of time.) 21

10 Molality of dissolved oxygen plotted as a function of time. 22

11 Molality of total calcium (solid), sulfate (dash-dotted), magnesium (dotted) and chloride (dashed) plotted as a function of time. 22

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Printed: April 30, 1997

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS: PCZ

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1 Computing Equipment ii

2 Initial fluid composition for major species corresponding to J-13 well water (Harrar et al., 1990). 4

3 Fluid composition for major species corresponding to UZ4-TP-3 (91.4 m) (Yang and Turner, 1988), and J-13 well water (Ogard and Kerrisk, 1984). 18

KTI: NEAR-FIELD ENVIRONMENT

Account Number: **20-5708-561**

Description: Near-field Environment Technical Assistance

Collaborators: Dr. M. Seth (Consultant)

Objective: Application of the computer code MULTIFLO, and submodules GEM and METRA to the Yucca Mountain HLW Repository.

1.30.96 *xx*-Repository Scale Calculation—Bounding Calculations

To derive bounds on some quantity it must first be determined how tight the bounds need to be, to be useful. Reasonable bounds are usually much more difficult to obtain than absolute bounds which are often overly conservative to be of much use. In the analysis which follows, pure evaporation, in which solute flux is assumed to be negligible, is analyzed.

Pure Evaporation The increase in concentration due to evaporation of water for a nonvolatile and nonreactive species such as chloride, assuming the aqueous solution remains undersaturated with respect to chloride-bearing minerals such as halite, can be easily calculated from the equation

$$m_i = \frac{n_i^0}{M_w^0 - n_w W_w}, \quad (1)$$

where m_i refers to the molality of the species in question, n_i^0 denotes the initial number of moles of that species in a given mass of water $M_w^0 = n_w^0 W_w$, n_w represents the number of moles of water evaporated, and $W_w = 0.018$ kg/mole- H_2O is the molecular weight of water. There are 55.51 moles of water in 1 kg. This relation is valid for a system which is closed with respect to the flux of liquid water into or out of the system. In particular, this same assumption applies to EQ6-type calculations. Shown in Figure 1 is a plot of Eqn.(1) for an initial mass of 1 kg water and an initial chloride concentration of 8 mg/kg- H_2O [compare with Figure 3.4-6 in the DOE report (Wilder, 1996) computed using EQ6].

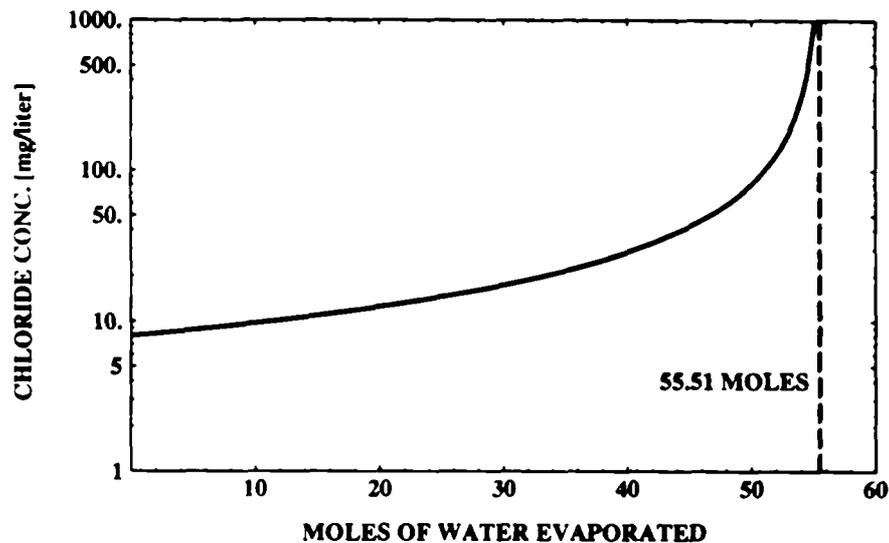


Figure 1: Increase in chloride concentration as water is evaporated from a container initially filled with 1 kg of water as described by Eqn.(1). To convert to molality note that 1000 mg/liter chloride is equivalent to 0.0282 molal.

To relate Eqn.(1) to the change in solute concentration in the near-field region of the repository, it is necessary to relate the number of moles of liquid water evaporated to the local value of the liquid saturation of the host rock. Provided the change in liquid saturation is caused by evaporation only, and not by the flux of liquid into or out of the control volume, liquid saturation s_l is related to the number of moles of water evaporated according to the equation

$$1 - \frac{s_l}{s_l^0} = \frac{n_w}{n_w^0}, \quad (2)$$

where the quantity n_w^0 represents the initial moles of water in a given volume of bulk rock, and s_l^0 refers to the initial liquid saturation. To obtain this equation note that liquid saturation is defined as the ratio of volume of liquid V_w to pore volume V_p

$$s_l = \frac{V_w}{V_p}, \quad (3)$$

and the liquid volume is related to the number of moles of water evaporated by the expression

$$V_w = (n_w^0 - n_w) \bar{V}_w, \quad (4)$$

with the initial volume of liquid given by $V_w^0 = n_w^0 \bar{V}_w$, and where \bar{V}_w denotes the molar volume of pure water. It follows that the molality is inversely proportional to

the liquid saturation

$$m_i = M_i^0 \frac{s_i^0}{s_i} \quad (5)$$

It is useful to define the enrichment factor η_i as the ratio of the concentration of some solute species at time t and location r , to the initial concentration at the same location. For a simple evaporative process, η_i is equal to the ratio of the initial saturation to the actual saturation

$$\eta_i = \frac{m_i}{M_i^0} = \frac{s_i^0}{s_i} = \frac{n_w^0}{n_w^0 - n_w} \quad (6)$$

According to this relation, the enrichment of some solute species due to pure evaporation is inversely proportional to the amount of water remaining in the control volume. If 90% of the water is evaporated, the enrichment factor for chloride is approximately 10 (Figure 1). As complete evaporation is achieved, the enrichment factor tends towards infinity. Clearly, at some point along the evaporation path when the aqueous solution reaches saturation with solid phases (salts), this relation must break down and the concentration becomes solubility limited.

2.7.97 Solubility Limit

A solubility-based estimate for the increase in chloride concentration resulting from evaporation may be derived by assuming the aqueous solution comes to equilibrium with a salt, e.g. halite. As evaporation proceeds, it is assumed that the sodium and chloride concentrations remain proportional to one another

$$a_{\text{Na}^+} = \alpha a_{\text{Cl}^-}, \quad (7)$$

with proportionality constant $\alpha \simeq 10$, as derived from J-13 well water (see Table 2). This is only correct if reaction with the solid phase does not remove sodium from solution. Equilibrium with halite implies the mass action equation

$$K = a_{\text{Na}^+} a_{\text{Cl}^-} = \alpha a_{\text{Cl}^-}^2 \quad (8)$$

Therefore

$$a_{\text{Cl}^-} = \sqrt{\frac{K}{\alpha}} \quad (9)$$

The $\log K$ for halite at 100°C is equal to 1.578, according to the EQ3/6 database (Wolery, 1992). (Note that because of vapor pressure lowering caused by capillary forces,

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the boiling point of water can be raised significantly above 96°C corresponding to the elevation of YM.) It follows that at this temperature the equilibrium activities for chloride and sodium are equal to $a_{Cl^-} = 1.945$ and $a_{Na^+} = 19.45$. This leads to an enrichment factor of roughly

$$\eta_{Cl^-} = \frac{C_{Cl^-}}{C_{Cl^-}^0} = \frac{1}{a_{Cl^-}^0} \sqrt{\frac{K}{\alpha}} \sim 10^4. \quad (10)$$

To obtain the actual concentrations, activity coefficient corrections must be applied. However, this result requires only that $\gamma_{Na^+} \approx \gamma_{Cl^-}$.

Table 2: Initial fluid composition for major species corresponding to J-13 well water (Harrar et al., 1990).

pH	6.8–8.3
Species	Molality $\times 10^3$
Ca ²⁺	0.290 – 0.370
Na ⁺	1.830 – 2.170
K ⁺	0.100 – 0.140
HCO ₃ ⁻	0.193 – 0.234
SiO ₂ (aq)	0.950 – 1.140
Cl ⁻	0.178 – 0.237

The chloride concentration in equilibrium with halite could be substantially increased if the sodium concentration is lowered by precipitation of other sodium-bearing solids such as feldspars. Thus this estimate could underestimate the chloride concentration. However, if halite saturation is never reached the predicted enrichment factor could be orders of magnitude larger than that which actually occurs in the repository. Equal concentrations of sodium and chloride in equilibrium with halite at 100°C implies roughly 6 M concentration of each species. Clearly, it is difficult to find a bound within reasonable limits even for a nonvolatile species such as chloride.

An estimate of the pH is more difficult to obtain and may depend on reactions with the host rock minerals as well as properties of the gas phase. Likewise, calcium and carbonate have no obvious bounds since their concentrations will be pH-dependent and will depend on reaction with calcite, for example.

2.21.97 Estimate of Chloride Concentration Based on MULTIFLO Calculations

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The computer code MULTIFLO (Lichtner, 1966; Lichtner and Seth, 1996b; Seth and Lichtner, 1996) provides a fully coupled, quantitative, description of two-phase fluid flow and reactive transport of aqueous and gaseous species. Heat flow is also accounted for in the code. The same complexity in chemistry is employed in MULTIFLO as in EQ6. The thermodynamic databases used by the two codes are equivalent. Fully coupled calculations using MULTIFLO are presented for the change in chloride concentration based on a repository-scale model. The repository is represented as a circular disk with a heat load of 83.4 MTU/acre. An initial saturation of approximately 80 percent throughout most of the unsaturated zone, becoming fully saturated at the water table, is assumed. For this case complete dryout does not occur. A single spatial dimension along the vertical through the center of the repository is considered. The repository horizon is located at a depth of 375 m from the surface.

The input files for GEM and METRA for use with versions 1.0 that are used in the calculations are listed below.

GEM:

```

Test Data for Multiflo Simulator (Yucca Mt., 1D, 83.4 AML)
      March 10, 1997
:
:      geometry nx  ny  nz   mode  iprint
GRID   XYZ      1   1 121   2     0
:
OPTS
:   idata  istart  imod  iexact
      0      0      10     0
:
:   itmax  ihalmax  ivmax  ndamp
      16     16     0     5
:
:   method  iops  ifor  isurf  iact  loglin  icon
      1      0     3     1     1     0     1
:
:   isync  ipor  iperm  perm-fac.
COUPLE  0     -1     0     3.
:
PLTFiles
:  iplot  a  s  t  m  si  sf  v  z  b  in  e  ex  ti  g  itex
      1   1  1  1  1  0  0  1  0  2  0  0  0  0  1  0
:
:   tol  ttol  tolneg  tolpos  tolexp  dthalf  qkmax  tolstdt
TOLR  1.d-10  2.e-3  1.e0  1.e-2  5.d0  .5  590.  1.e-12
:
:   mcyc  cc  c  flx  r  sp  qk  pk  rk  a1  a2  a3

```

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Printed: April 30, 1997

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS: PC

```

DEBUG 0 1 1 0 1 1 1 1 1
:
: isat isothrm iread por0 phir sat w lambda toldelt tolpor
ISYSTEM 0 1 0 .11 1. 0.5 .5 1. 1.e-3 1.e-3
:
: vx0 vy0 vz0[m/yr] alphax alphas alphaz cournr
FLOW 0. 0. 1. 0. 0. 0. 1.
:
: d0[cm^2/s] delhaq[kJ/mol] dgas[cm^2/s] dgexp tortaq tortg idif
DIFF 1.d-5 12.6 2.13d-1 1.8 1.d0 1.d0 0
:
:flag 1: T(x) = d x^3 + a x^2 + b x + c (meters)
: 2: T(x) = a + (b-a) exp[-((x-x0)/c)^2] + (d - a) * x / xlen
: 3:T(x,t)=a+1/2(b-a)(erf[(x+c-x0)/2sqr(dt)]-erf[(x-c-x0)/2sqr(dt)])
: p (bars) temp flag a b c d x0 xlen
PTINit 1.0 25. 0 25 300 250 125 1000. 2.d3
:
:master species for controlling time stepping
MASTER h+
:
:grid m 0. 1 200 200.
:
DXYZ
1.
1.
121*1.
:
: isolv level north nitmax idetail rmaxtol rtwotol smaxtol
SOLV 3 1 1 100 0 1.e-20 1.e-20 1.e-12
:
:initial and boundary conditions: 1-conc., 2-flux, 3-zero gradient
:inlet outlet nzoneaq
COMP 1 3 3
:
:species itype guess ctot mineral diffusion
ca+2 1 4.e-4 4.e-4 blank 0.8e-5
na+ 1 2.e-3 2.e-3 blank 0.8e-5
h+ 8 1.e-8 8.0 blank 9.6e-5
hco3- 4 2.7e-3 -2.99 co2(g)
sio2(aq) 1 2.e-3 2.e-3 blank 0.8e-5
cl- -1 2.e-3 2.e-3 blank 0.8e-5
:blank
:
BCON
3 3
:species itype guess ctot mineral
ca+2 1 4.e-4 4.e-4 blank
na+ 1 2.e-3 2.e-3 blank
h+ 8 1.e-8 8.0 blank
hco3- 4 2.7e-3 -2.99 co2(g)
sio2(aq) 1 2.e-3 2.e-3 blank
cl- -1 2.e-3 2.e-3 blank
:

```

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Printed: April 30, 1997

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS: PCZ

```

4 3
:species  itype  guess  ctot  mineral
ca+2      1      4.e-4  4.e-4  blank
na+       1      2.e-3  2.e-3  blank
h+        8      1.e-8  8.0    blank
hco3-     4      2.7e-3  -2.99  co2(g)
sio2(aq)  1      2.e-3  2.e-3  blank
cl-       -1      2.e-3  2.e-3  blank
:
0 0
:
CMIR  0  0
      :blank
:
STOL  1. 1. 1. 1. 1. 1. 1. 1.
:
AQCX
oh-
co2(aq)
co3-2
caco3(aq)
cahco3+
caoh+
cacl+
cacl2(aq)
nahco3(aq)
nacl(aq)
naoh(aq)
h3sio4-
h2sio4-2
      :blank
:
MNRL
crystalite
quartz
chalcedony
calcite
tobermorite-14a
halite
      :blank
:
GASEs
co2(g)
      :blank
:
MNIR
:mineral  itypkin  fkin  delh  beta  rka  betb  rkb  rk  tau
: i1 i2 j1 j2 k1 k2 vol area
crystalite 0 1.0 75. 1.0 0. 1.0 0. -16.34 1.e-3
1 1 1 1 1 121 0.14 1.e1
0
quartz      0 1.0 75. 1.0 0. 1.0 0. -17.39 1.e-3
1 1 1 1 1 121 0.14 1.e1

```

P. C. Lichtner

SCIENTIFIC NOTEBOOK

INITIALS: PCZ

```

0
chalcedony  0  1.0  75.  1.0  0.  1.0  0. -30.39  1.e-3
1 1 1 1 1 121  0.61  0.e1
0
calcite      0  1.0  35.  1.0  0.  1.0  0. -10.00  1.e-4
1 1 1 1 1 121  0.  1.
0
tobermorite-14a 0 1.0  30.  1.0  0.  1.0  0. -12.00  1.e-4
1 1 1 1 1 121  0.  10.
0
halite       0  1.0  30.  1.0  0.  1.0  0. -12.00  1.e-3
1 1 1 1 1 121  0.  10.
0
:blank
:
:surface mineral itypkin area beta fkin delh rkph rk
:  0 1.0 1.0  1. 0.  0.  0.
:
:corrosion solids i0 acorr bcorr curlim
:  0. 0. 0. 0.
:
:crevice gap[meters] potential [v]
ECAQ  90.d-6  .2
:blank
:
:electrochemical aqueous species i0 acorr bcorr curlim
:  0. 0. 0. 0.
:
AQIR
:blank
:
:ion-exchange reactions
Ionx  0  1.0
:
BRKP  1
72
:
DTStep[y]  1 3.e-8
1.e-8  100.d0
:
TIME[y] 8 10. 50. 100. 500. 1000. 5000. 10000. 1.e5
:
ENDS

```

METRA:

Data for Multiflo simulator (initial data : 2D, 83.4 AML, Yucca Mt.)
Dec. 27, 1996

```

RSTART  0
:
: XYZ = 1 table look-up, pref = ref. press.
: RADIAL = 0 correlations, tref = ref temp.

```