

1/27

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

CORRECTIVE ACTION REQUEST

CAR No. 93-4 Associated AR,SR,NCR NO. 93-13

PART 1: DESCRIPTION OF CONDITION ADVERSE TO QUALITY

Contrary to the requirements of QAP-001, Rev. 1, "Scientific Notebook Control," and QAP-014, "Documentation and Verification of Routine Calculations," errors in the documentation of initial and in-process entries were noted in eleven of fourteen scientific notebooks reviewed. Typical errors include: No title or clear objectives identified, prerequisites not identified and/or noted as being verified, no indication that computer output was verified, and entries not signed or dated. See Surveillance Report 93-13 for a complete list.

Initiated by: Rw Welch Date: 11/11/93
PART 2: PROPOSED ACTION Responsible Element Manager: Budhi Sagar

a) Root Cause:
lack of formal training

b) Corrective Action to Preclude Recurrence:
Train the modelers in the use of this procedure

Target Date for Completion: Dec. 15, 1993

Response provided by: Ranjit Sofen Date: 11/24/93

PART 3: APPROVAL
Comments/Instructions: ON 11/24/93 A SCIENTIFIC NOTEBOOK TRAINING SESSION WAS HELD AT THE CNWRA FOR 14 MODELERS, SEE ATTACHED ATTENDANCE LIST AND A COPY OF THE VIEWGRAPHS UTILIZED. INITIAL FEEDBACK WAS GOOD. COPIES OF "GOOD EXAMPLES" WILL BE MADE AND DISTRIBUTED TO ALL CNWRA MODELERS.

Director of QA: Suman Mahanta Date: 12/3/93

PART 4: VERIFICATION OF CORRECTIVE ACTION IMPLEMENTATION
TRAINING ACCOMPLISHED. FOLLOW UP MEMORANDUM SENT OUT. SEE ATTACHED DOCUMENTATION. A SECOND MEMORANDUM WAS SENT OUT 1/6/94 WHICH CONTAINED THE VIEWGRAPH COPIES USED IN THE ORIGINAL QAP-001 TRAINING. SEE ATTACHED.

Verified by: Suman Mahanta Date: 1/6/94

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

MEMORANDUM

January 6, 1994

TO: Ron Martin Steve Young Ron Janetzke
 Chuck Connor David Turner Gustavo Cragnolino
 John Hageman Simon Hsiung Pat LaPlante
 N. Sridhar Hengameh Karimi Goodluck Ofoegbu
 Berge Gureghian

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

SUBJECT: Tips for Maintaining Your Scientific Notebooks

REFERENCE: Scientific Notebook Control Requirements (QAP-001)

Recently you received a memorandum from me which identified "Scientific Notebook Good Practices," dated 12/17/93. The examples cited came from a few specific CNWRA staff members who maintain their Scientific Notebook(s) in accordance with Quality Assurance Procedure-001.

The purpose of this memorandum is to reemphasize the importance of complying with the requirements of QAP-001 and to provide you copies of the viewgraphs utilized in the 11/24/93 Scientific Notebook training.

If you have any questions regarding your Scientific Notebook(s) or application of QAP-001 to your numerical modeling, contact Bob Brient at ext. 5537 or me at ext. 5149.

cc: W. Patrick
 B. Sagar
 Element Managers
 R. Brient
 QA Records/CAR 93-4 Folder



CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES QUALITY ASSURANCE SURVEILLANCE REPORT

PROJECT NO.: 20-5702-154 REPORT NO.: 93-13 PAGE 1 OF 2

SURVEILLANCE SCOPE:
Fourteen scientific notebooks were selected to verify compliance to applicable procedural requirements. Thirteen of the fourteen notebooks reviewed were being used primarily for software development and analysis activities. Initial entries, in-process entries, and documentation of routine calculations were evaluated.

REFERENCE DOCUMENTS:
QAP-001, Revision 1, "Scientific Notebook Control"
QAP-014, Revision 0, "Documentation and Verification of Routine Calculations"

STARTING DATE: October 22, 1993 ENDING DATE: October 27, 1993
QA REPRESENTATIVE: R. W. Folck, SwRI Institute QA *RW Folck*

PERSONS CONDUCTING TEST/EXAM/ACTIVITY:
David Turner Ross Bagtzoglou Jose Menchaca Bill Murphy
Gordon Wittmeyer Renner Hofmann Steve Young Randall Manteufel

SATISFACTORY FINDINGS:
Three of the fourteen scientific notebooks were found to be in general compliance with procedural requirements. One notebook was found to contain only minor data entry errors, (e.g. missed initial and date). See Page 2 for noted good practices.

UNSATISFACTORY FINDINGS:
Errors were noted in eleven of the fourteen scientific notebooks selected for review. See Page 2 for a list of typical discrepancies.
NONCONFORMANCE REPORT NO.: CAR 93-4

ATTACHMENTS: none

RECOMMENDATIONS/ACTIONS

- In-process review of notebook(s) by immediate supervisor.
- Review applicability of procedural requirements to software development and analysis activities.
- Assign a scientific notebook to only one definable function, task, or computer code.

APPROVED: *[Signature]*
CENTER DIRECTOR OF QUALITY ASSURANCE
DATE: 11/15/93

DISTRIBUTION:
ORIGINAL - CENTER QA DIRECTOR
ORIGINATOR
PRINCIPAL INVESTIGATOR - R. Manteufel/R. Green
ELEMENT MANAGER - B. Sagar/R. Baca
Distribution AT CNWRA to all Directors/Emgs.

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Satisfactory Findings:

- Entries made on a regular basis.
- Data file downloaded onto diskette and secured in notebook.
- Charts secured with tape and the boundary initialled and dated.
- Signatures and initials documented on first page of notebook.
- Title, scope, and objectives clearly documented as headers.
- Index developed for notebook entries and structure.
- Entries generally readable and in ink.

Unsatisfactory Findings:

Initial Entries:

- No title or clear objectives identified.
- The equipment, e.g. computer, to be used was not specifically identified. Model numbers were not noted as well as operating system(s).
- No special training or qualification requirements. Summer students were used on several tasks.
- Potential source of uncertainty or error not identified.

In-process Entries

- Prerequisites not identified and/or noted as being verified.
- References made to future events were unverifiable, e.g. Codes will be copied.
- Referenced documents not verifiable. SPR noted without corresponding number. Report without corresponding date or number.
- Entries indicate satisfactory testing without supporting test data.
- Reference made to test data on local hard drives and on LAN.
- Test I/O included but, no reference as to "how" testing was done. Test procedure not documented.
- No indication that output was evaluated or checked.
- Code version numbers under test or analysis not documented.
- Calculations performed by spreadsheet not verified by hand calculation.
- Step-by-step process of the analysis not clear. Unable to determine how conclusions were derived.
- Data entries made without supporting description or explanation.
- Notebooks used as journals/diaries to document meetings, schedules, time accounting, etc.

Documentation

- Entries not signed or dated.
- Corrections not made with single line, initialled, and dated.
- "White-out" used.
- Same notebook copy number issued to two different individuals. Corrected during surveillance.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES MEETING ATTENDANCE

SUBJECT OF MEETING *QAP-001 Scientific Notebook Control Training*

DATE: *11/24/93*

LOCATION: *CNWRA Conference Room # 1*

PERSON	ORGANIZATION	TITLE/FUNCTION	TELEPHONE NUMBER
<i>Robert G. Baca</i>	<i>CNWRA</i>	<i>EM PA</i>	<i>3805</i>
<i>SOV SPONTOFF</i>	<i>"</i>	<i>RES SCI PA</i>	<i>5203</i>
<i>William Murphy</i>	<i>CNWRA</i>	<i>Principal Scientist</i>	<i>5263</i>
<i>Sitakanta Mohanty</i>	<i>CNWRA</i>	<i>Res. Sci., PA</i>	<i>5185</i>
<i>Robert Briert</i>	<i>CNWRA</i>	<i>Res. Sci.</i>	<i>5537</i>
<i>Randy Folck</i>	<i>Institute QA</i>	<i>QA Engr.</i>	<i>2951</i>
<i>VIVEK KAPOOR</i>	<i>CNWRA</i>	<i>RESSCI</i>	<i>2470</i>
<i>POSS BAPTISTON</i>	<i>"</i>	<i>SRE</i>	<i>5182</i>
<i>Jose M. Menchaca</i>	<i>Div 15</i>	<i>Sr Research Scientist</i>	<i>3860</i>
<i>Renner B. Hofmann</i>	<i>CNWRA</i>	<i>sr Res. Scientist</i>	<i>5388</i>
<i>BRITAIN HILL</i>	<i>"</i>	<i>RESEARCH SCIENTIST</i>	<i>6087</i>
<i>Gordon Wittmeyer</i>	<i>"</i>	<i>Sr Res. Sci.</i>	<i>5082</i>
<i>Ron Green</i>	<i>"</i>	<i>"</i>	<i>5305</i>
<i>Aaron DeWispelan</i>	<i>"</i>	<i>Prin Engr</i>	<i>6072</i>
<i>Randall D. Mantel</i>	<i>"</i>	<i>Res. Engr.</i>	<i>5250</i>
<i>Peter Lichtner</i>	<i>CNWRA</i>	<i>Principal Sci</i>	<i>6084</i>
<i>Bruce MAGRITO</i>	<i>"</i>	<i>Director QA</i>	<i>5149</i>

QAP-001 SCIENTIFIC NOTEBOOK CONTROL TRAINING

- WHY THIS TRAINING?
 - SURVEILLANCE 93-13, CORRECTIVE ACTION REQUEST 93-4
- OBJECTIVE: COMPLIANCE WITH QAP-001; FEEDBACK FROM MODELERS
- SURVEILLANCE FINDINGS:
 - 3 OF 14 SCIENTIFIC NOTEBOOKS FOUND IN GENERAL COMPLIANCE WITH PROCEDURE
 - CAR 93-4 ISSUED TO ADDRESS 11 OF 14 NOTEBOOKS IN NON-COMPLIANCE
 - GOOD PRACTICES
 - UNSATISFACTORY PRACTICES

*copy of 6
Micrographs
used in Training
BSC*

WHY SCIENTIFIC NOTEBOOKS?

- CONTRACT NRC-02-88-005 STATES:

"E.2 QUALITY ASSURANCE - ALL WORK (I.E. DATA COLLECTION, ANALYSES, COMPUTATIONS, METHODS, ETC.) CONDUCTED UNDER THIS CONTRACT SHALL BE PERFORMED IN ACCORDANCE WITH AN ACCEPTED QUALITY ASSURANCE PROGRAM ADDRESSING THE CRITERIA OF 10 CFR PART 50 APPENDIX B, AS APPROPRIATE, AND THE GUIDANCE OF THE NRC REVIEW PLAN FOR THE HLW QA PROGRAM DESCRIPTIONS APPLICABLE TO RESEARCH AND TECHNICAL ASSISTANCE..."

CENTER QUALITY ASSURANCE MANUAL

3.7.2 CONTROL BY SCIENTIFIC NOTEBOOK METHOD

"THE PRINCIPAL INVESTIGATOR FOR THE EXPERIMENTAL TASK SHALL DEVELOP AND MAINTAIN THE SCIENTIFIC NOTEBOOK."

"THE SCIENTIFIC NOTEBOOK PROVIDES HISTORICAL DOCUMENTATION OF THE ... TASK INCLUDING PLANNING, DESIGN OF EXPERIMENTS (IF APPLICABLE), CONTROL OF EXPERIMENTS/TESTS, AND DOCUMENTATION OF RESULTS."

QAP-001 SCIENTIFIC NOTEBOOK CONTROL TRAINING

- EACH PI SHOULD HAVE HIS/HER CONTROLLED QAP-001 PROCEDURE
- SPECIFIC GUIDANCE CONTAINED THEREIN
- PIs RESPONSIBLE FOR IMPLEMENTATION OF QAP-001
- COGNIZANT EMs RESPONSIBLE FOR OVERALL IMPLEMENTATION OF QAP-001

SURVEILLANCE NOTED GOOD PRACTICES

- REGULAR (PERIODIC) ENTRIES
- DATA FILES DOWNLOADED TO DISKETTES & SECURED IN NOTEBOOK
- CHARTS TAPED AND BOUNDARY INITIALLED/DATED
- SIGNATURES/INITIALS DOCUMENTED ON NOTEBOOK FIRST PAGE
- TITLE, SCOPE, OBJECTIVES CLEARLY DOCUMENTED
- INDEX DEVELOPED FOR NOTEBOOK ENTRIES/STRUCTURE
- ENTRIES GENERALLY READABLE AND IN INK

SURVEILLANCE UNSATISFACTORY FINDINGS - **INITIAL ENTRIES**

- NO TITLE OR CLEAR OBJECTIVES IDENTIFIED
- COMPUTER TO BE USED NOT IDENTIFIED
- COMPUTER MODEL/NUMBERS/OPERATING SYSTEM(S) NOT NOTED

SURVEILLANCE UNSATISFACTORY FINDINGS **IN-PROCESS ENTRIES**

- REFERENCES TO FUTURE EVENTS UNVERIFIABLE ("CODES WILL BE COPIED")
- REFERENCE DOCUMENTS NOT VERIFIABLE (SPR NOTED W/O NUMBER)
- CODE TESTING WITHOUT SUPPORTING DATA
- REFERENCE MADE TO TEST DATA ON LOCAL HARD DRIVES/LAN
- TEST I/O INCLUDED, NO REFERENCE AS TO HOW TESTING WAS DONE

SURVEILLANCE UNSATISFACTORY FINDINGS - IN-PROCESS ENTRIES

- CODE VERSION NUMBERS UNDER TEST NOT DOCUMENTED
- STEP-BY-STEP PROCESS OF ANALYSIS NOT ALWAYS CLEAR
UNABLE TO DETERMINED HOW CONCLUSIONS WERE DERIVED
- DATA ENTRIES LACK DESCRIPTION
- NOTEBOOKS USED TO DOCUMENT UNRELATED WORK

QAP-014 DOCUMENTATION AND VERIFICATION OF ROUTINE CALCULATIONS

- NO INDICATION OUTPUT WAS EVALUATED OR CHECKED
- CALCULATIONS PERFORMED BY SPREADSHEET NOT VERIFIED

SURVEILLANCE UNSATISFACTORY FINDINGS - DOCUMENTATION

- ENTRIES NOT SIGNED/DATED
- CORRECTIONS NOT MADE WITH SINGLE LINE, INITIALED/DATED
- "WHITE OUT" USED
- SAME NOTEBOOK COPY NUMBERS ISSUED TO 2 DIFFERENT INDIVIDUALS

QAP-001 SCIENTIFIC NOTEBOOK CONTROL TRAINING

- QUESTION OF CNWRA NOTEBOOK CONSISTENCY ACROSS ELEMENT
- INPUT TO QAP-001 PROCEDURE FROM MODELERS

SENT out 12/17/93
EE

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 16

MEMORANDUM

December 17, 1993

TO:

W. Murphy	S. Stothoff	S. Mohanty	V. Kapoor
R. Bagtzoglou	J. Menchaca/Div 15	R. Hofmann	B. Hill
G. Wittmeyer	R. Green	A. DeWispelare	R. Manteufel
P. Lichtner	R. Martin	S. Young	R. Janetzke
C. Connor	B. Gureghian	G. Cragolino	H. Karimi
J. Hageman	S. Hsiung	P. LaPlante	N. Sridhar
G. Ofoegbu	D. Turner		

FROM: Bruce Mabrito, Director of Quality Assurance



SUBJECT: Scientific Notebook Good Practices

In the Scientific Notebook Control Training class held November 24, 1993, it was noted that in addition to the unsatisfactory findings identified in Surveillance Report No. 93-13, there were numerous good practices observed. The purpose of this memorandum is to provide that objective evidence (attached) to those individuals who regularly utilize scientific notebooks in the course of their software development and analysis activities.

As you review these examples of proper compliance with Quality Assurance Procedure-001, Scientific Notebook Control, please note that the general topic shown (such as "Signatures and Initials of notebook users") is in the upper left hand corner of each page.

If you have any questions regarding application of QAP-001 to software development and analysis activities, please call me at ext. 5149.

cc: W. Patrick
Directors
Element Managers
R. Brient
G. Stirewalt
D. Ferrill
CAR 93-4 File

*Signatures and Initials of notebook users.



account book S149

Available in 150 and 300 pages

Michael A. Muller

Michael A. Muller M.M.

Ross Bagtonglan

Ross Bagtonglan
RB



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Documentation

Primary documentation of the software consists of the software itself, which is heavily documented internally. Formal documentation is in preparation at LLNL.

Documentation for individual uses of the codes will consist of the reports in which results are presented, together with references to the versions of the codes used. Code versions will be documented in this book.

WMP 5/14/92

Primary source

The EQ3/6 software package has been under development and control at Lawrence Livermore National Laboratory (LLNL) for over a decade. Versions of the codes and data bases issued directly from them are the primary source.

Two primary packages have been officially received at the CNWRA. They are referred to at the CNWRA as the EQ3/6-90 package and EQ3/6-92 package. The later is an update of the former. Both were transferred by FTP to the CNWRA.

The EQ3/6-90 package was copied unmodified onto two 3 1/2" diskettes labelled EQ3/6 Codes 1/3/91 Diskettes 1 and 2, 91-15, and have serial numbers A4DF:6814 and A507:CC14.

The EQ3/6-92 package was copied onto two diskettes labelled EQ3-6 Feb 1992 release 1 and 2 with ^{no} serial numbers on the disks.

WMP 5/14/92

Primary source, cont.

The four diskettes constitute the primary source and are in storage in the locked file cabinet at the CNWRA.

In addition to the disks, copies of the materials received from LLNL were placed in the CTCVAX account of William Murphy (account WMM) at SWRI. Other copies were made from this material and distributed among researchers at the CNWRA and elsewhere. Modifications made to these materials are to be recorded in this book or otherwise documented if the resulting software is used to develop products for the NRC.

WMM 5/14/92

Software in use

Use of the EQ3/6 software involves the codes EQ6, EQ3NR, EQUB, and EQPT, plus one or more data bases. (EQ3RR is colloquially referred to as EQ3).

The EQ3/6-90 package contained the following versions of software:

EQ3NR	3245R124
EQ6	3245R119
EQUB	3245R153
EQPT	3245R80

The EQ3/6-92 release consists essentially of updated versions of these codes and data bases with corrected bugs, etc. The LLNL practice is to designate modified or updated versions as with an "X". The -90 package contains the following versions:

EQ3NR	3245R124X
EQ6	3245R119X
EQPT	3245R80X
EQUB	3245R153

WMM 5/14/92

Modifications for use at SwRI

Minor modifications to the codes are required to enable their use on the SwRI CCFVAX. These are outlined below:

EQ3; EQ6; EQLIB; EQPT:

The only modifications are to eliminate calls to machine dependent clocks and replace them with calls to the SwRI VAX clock subroutine. This permits printing of the time and date of each run on the run output, and in no way affects any scientific calculations.

Modifications to codes are generally labelled in the codes by documentation (comment lines). Modifications by Murphy are labelled in comments by the name MURPHY, and are generally in upper case.

WMM 5/15/92

Modified codes have been given new stage numbers as listed below. These versions of the codes are in general use at the CNWRA.

EQ3NR	3245R124xWM
EQ6	3245R119xWMM
EQPT	3245R80xMUR
EQLIB	3245R153xMUR

WMM 5/15/92 These versions of the codes, ^{will be} ~~have~~ been copied on diskettes and ^{will} placed in storage in the locking file cabinet at the CNWRA. 5/15/92

WMM 5/15/92

An additional modification to EQLIB was made in the call statement for the data base. Restricting the call statement to "read only" permits all users on different accounts at the CNWRA to access one controlled version of the data bases.

WMM 5/26/92

EQ3/6 software data exemption memo attached WMM 5/15/92

~~Bill Murphy~~ 21

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

Memorandum

To: Wesley C. Patrick (Technical Director)
and Bruce E. Mabrito (Director of Quality Assurance)

From: William M. Murphy *WMM*

Re: Exemption for qualification of data in the EQ3/6 software package

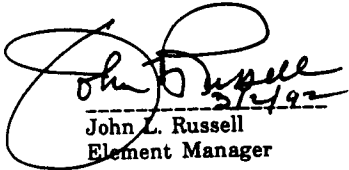
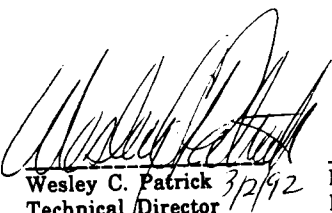
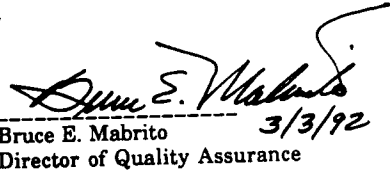
Date: March 2, 1992

The EQ3/6 software package for geochemical modeling is under continuing development by the Department of Energy at Lawrence Livermore National Laboratory. Versions of the EQ3/6 software package have been and will be employed in research and technical assistance activities at the Center for Nuclear Waste Regulatory Analyses. The package includes several data bases of thermodynamic properties for species and reactions. The purpose of this memorandum is to petition for exemption of these existing data from qualification requirements under Quality Assurance Procedure QAP-015.

Several criteria in QAP-015 permit and justify the exemption. Section 5.1.3 states that it is unnecessary to evaluate data if "The existing data were generated by the DOE or its contractors and the purpose of the Center activity or project is to provide an independent evaluation of that data." Section 5.1.3 also states that qualification is unnecessary if "The existing data are being used as a basis of comparison in confirmatory research or other evaluations." The EQ3/6 compilations of existing data were generated by the DOE, and one purpose of all CNWRA uses of the EQ3/6 data is to provide independent evaluation and confirmation.

Regarding use of EQ3/6 data for other than strict evaluation and confirmation, Section 5.3 of QAP-015 permits exemption from data qualification under circumstances where "Programmatic requirements and constraints or other factors may make it necessary to use data which are not qualified." Progress in numerous research and technical assistance activities at the CNWRA requires the use of geochemical data. Many data in the EQ3/6 data base fall in the category of "information which is accepted by the scientific and engineering community as established facts," and is therefore not "existing data" in the context of QAP-015 (Section 4.3). Other data in the EQ3/6 package are recognized by the scientific and engineering community as speculative. However, they represent the current and evolving state of the art in geochemical data. While activities at the CNWRA may address the state of the art in geochemical data in narrowly defined areas, it is beyond the scope of the CNWRA program and resources to do so for all data in the EQ3/6 package, which includes data for over 1700 species.

Concurrence Approval Approval

 John L. Russell Element Manager	 Wesley C. Patrick Technical Director	 Bruce E. Mabrito Director of Quality Assurance
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* Referenced Document stapled in notebook.

Handwritten notes at the bottom of the page, including "EQ3/6" and other illegible scribbles.

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5/31 - 6/4 Worked on the Study Plan review.
Also started work on the CDS.

6/7 - 6/11 Finalized Study Plan review.

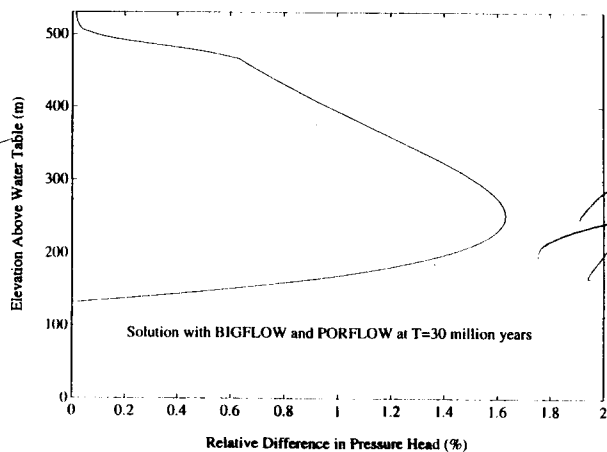
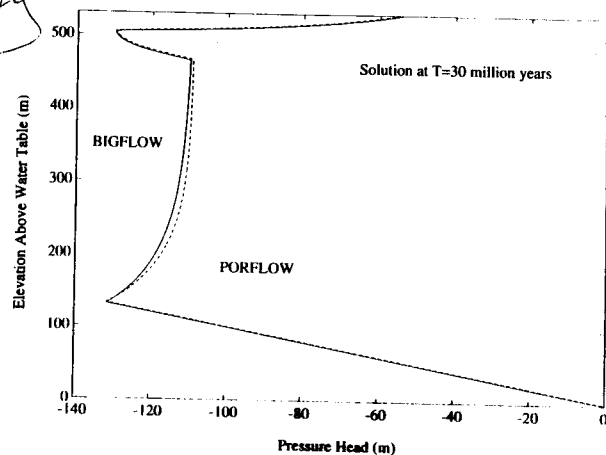
Started work with Ashok and Rashid on modifying BIGFLOW. Changes are made to optimize the code (loop control) for all possible cases of flow conditions.

Rashid indentified some extremely unstable material which led to some efficiency loss. It did not, however, affect the solution. Simulations were conducted on the COVE-2A test case (SAND89-2558) for benchmarking the new version of BIGFLOW for a realistic case. Data representative of Yucca Mountain were used. It was found that close to steady-state solution is obtained after about 31 million years. This concluded also the verification of BIGFLOW (version with fully heterogeneous Van Genuchten "n").

Comparisons with PORFLOW are shown on the next page. The maximum relative error observed is at a depth of ≈ 300 m and is $\approx 1.5\%$. This is assuming that the PORFLOW solution is correct.

Worked also on CDS 3.2.2.6. Had telecon meeting on Friday with Bill Ford, Neil Coleman, and Dave Books. Finally, worked with Steve Seida on the AMN project.
(cont'd)

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4

3/26 Latest version of "ET" CDS received, late Friday. Will review on Monday.

Meeting w/ M. Muller next cell. Very interesting results. GLFRAC3D is indeed a useful tool for visualizing complex 3D fracture sets. Outcrops are nicely demonstrated, plane intersections, and line connections. CPU time requirements are rather extensive, especially for the full set (205 fractures).

Discussion and extensive probing revealed potential small problem with the size of the domain. This leads to having much more line connections and plane intersections, than we have. Mike Muller will look into this.

3/29 final version of BIGFLOW manual is getting close to being done. Working on figures and flowcharts.

Visualization "bug" is being eliminated. "ET" CDS being reviewed. Comments were forwarded to Mike Miklas.

Variogram 3D code is fully coupled with NNM code. Analysis revealed a preliminary "correct" structure in terms of λ (correlation length). Some questions regarding σ_y are to be resolved.

5

3/30 Visualization code is almost complete in its revised form. Dry-run is to be conducted and decision on which figures to present during the mid-year review is needed.

Work on the IRFD project (fuzzy set phase) re-started. Running of CMVSFS (connection Mapping) code for verification purposes. The problem is 2D with an obstacle (of conductivity). Description of the problem is presented in the Progress Report #1 (1/24/92) to the ACR Committee.

Further analysis with CMNNM continues. Repeated unconditional realizations are being analyzed to get a better insight regarding geostatistics.

3/31 Worked with Mike Muller on the visualization of fracture results. Decided on which figures to present in slide mode. Will take pictures tomorrow. Had a discussion with Mike Miklas re: the "ET" CDS. Our review of Neil Glenan's work is consistent. Will talk with Neil tomorrow.

Worked with Sitkanta on the NNM code. Verified that the generator is working OK in terms of variogram. The correlation length is a bit off. $\lambda = 5.9$ specified vs. $\lambda \approx 7$ fitted but the variogram is a beautiful exponential. Remember, also, that the variogram plotted is the mean of 10 realizations, i.e. σ_y . The potential "bug" regarding the std is still there.

3/25

Running program mdmf under the title mdmv.p. input files INPUT & INDATA.

- Gives segmentation violation prob when a field of size 16x16x16 is used on rebarian
- Therefore, currently 9 trials are trying it on ~~the~~ vax 8700.

3/26

work done for Gordon

PORFLOW version 2.4.1 was tested on sparc machine (rebarian). The particular version that was used did not reproduce the results for prob 1 in the manual (NUREG/CR-5991)

Need to get a new version and test it on VAX before transferring to sparc. The above problem may answer questions regarding the strange answers we are obtaining on a one-D unsat flow problem

3/26

A code "variogram3d.f" was developed to determine the variograms in three different directions of a 3-D field. This is a modification of variogram2d.f which was formerly named as variogram.f. The field was generated by using GSLIB program

me
me 2
993

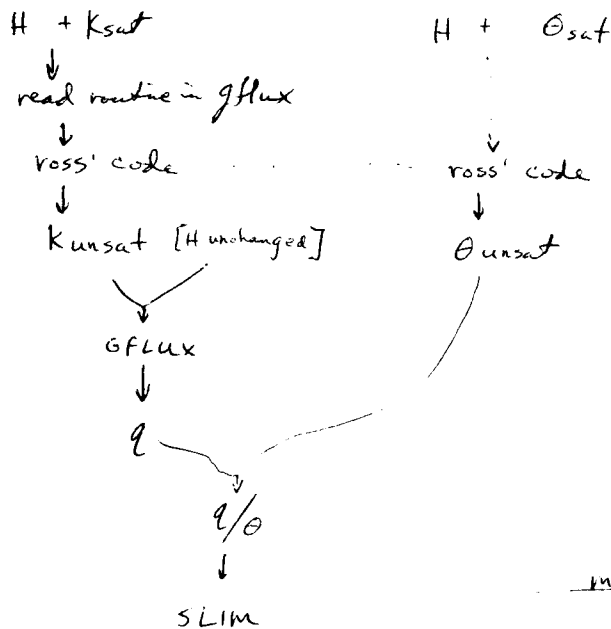
Ran flowproc with byflow files
HEAD-TI and KSAT, blew up.
Looked at GFLUX sub-part of
flowproc. Updated ross a little mm.

~~Wed~~ Thurs
June 3
1993

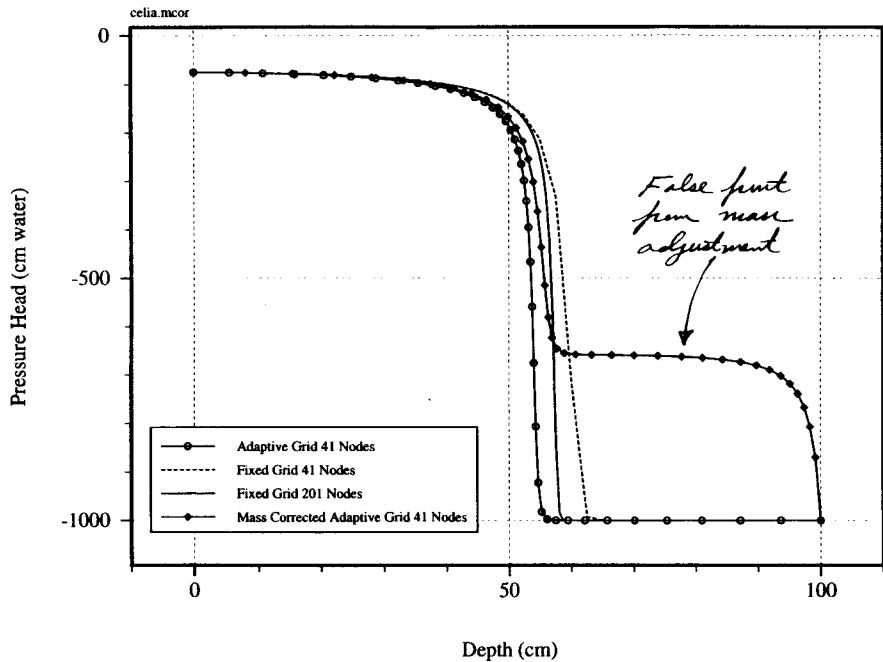
Met w/ Ross, talked about what to do.
Ran flowproc, found error.

HEAD and KSAT file did not have the same
header FXXL1,2,3 was different. Program
should still run with these different but
it doesn't so I edited HEAD file to
match KSAT file - ran OK

Here is process

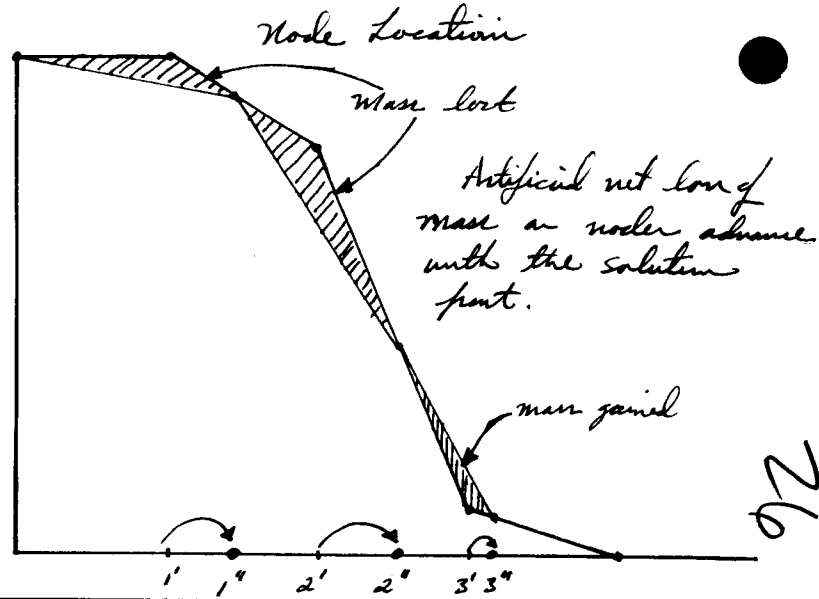
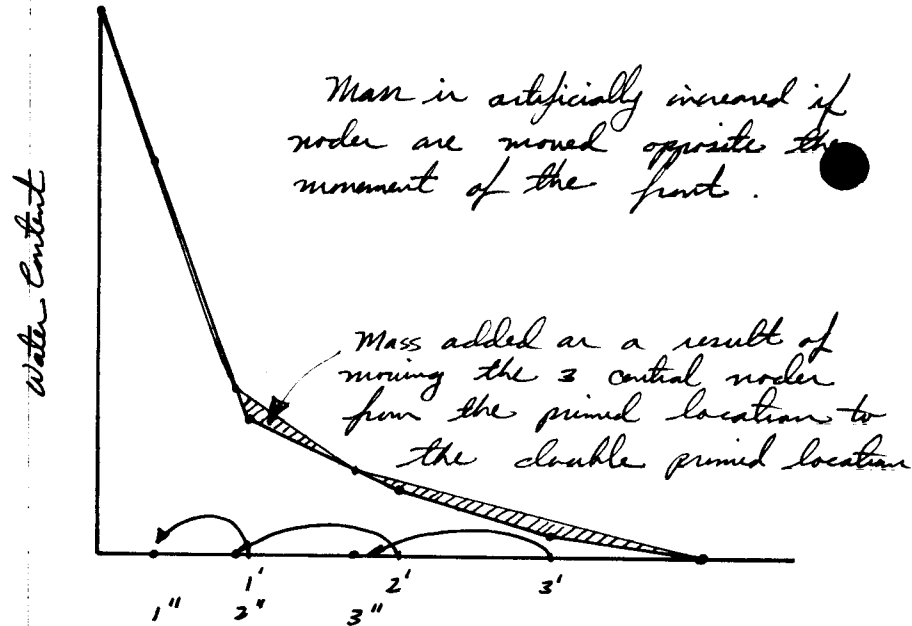


Pressure Heads from ADAVAR



The reason for mass balance error arising due to the process of grid mapping may be demonstrated by a simple graphing exercise. ➡

Front Movement →



* Input/Output

The test case used here considers flow in matrix only.

Input data file for ADAVAR:

```

2 0 0 2 1 1 1
1.000d+00 1.000d+00 1.440d-02 1.100d+00 1.001d+13
5.000d-08 20 40 1 1 1.000d+12 0 1
1.001d+13
0.000d+00 1.000d+13
1.001d+13
530.4d+0 5 1.5d+1
8.210d-03 8.000d-02 1.600d-04 1.558d+00 1.000d-07 9.700d-12
1.500d-02 4.000d-01 4.000d-02 8.872d+00 1.000d-07 3.900d-07
5.870d-03 1.100d-01 8.800d-03 1.798d+00 1.000d-07 1.900d-11
5.870d-03 1.100d-01 8.800d-03 1.798d+00 1.000d-07 1.900d-11
1.800d-02 4.600d-01 1.888d-02 3.872d+00 1.000d-07 2.700d-07
530.4d+0 503.6d+0 25
503.6d+0 465.5d+0 25
465.5d+0 335.4d+0 25
335.4d+0 130.3d+0 25
130.3d+0 0.0d+0 25
-1.000d+02
2 1
-3.170d-12 -3.170d-12
0.000d+00 0.000d+00
    
```

1 ⇒ SS
 0 ⇒ Transient
 0 ⇒ Resist loss
 0 ⇒ Non-adapt. for TR
 1 ⇒ resist. for TR
 2 ⇒ resist. for TR

These are
 Sr not Or !!

→ infiltration rate at
 top = .1 mm/yr

Material Props.
for layer 1-5

Top & Bottom
Elev. of layer
1-5

Results for steady-state run and transient run to steady state

