

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

1/4 5/8
JH
6-6-95

NONCONFORMANCE REPORT

Project No. 20-5702-523

NCR No. 94-03

PART 1: DESCRIPTION OF NONCONFORMANCE

Supervision 93-11 identified the following deficiencies in MARIANA & TWITCH code

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1. INEL listings for MARIANA state that it is Version 2.0 while Software Summary Form states it is Version 1.0 (TOP-018, para. 5.4).
2. No objective evidence that the software tools PREFOR, FORWARN, CRAFT, and PCMetrics had been executed (TOP-018, para. 6.3.1).
3. No objective evidence found to indicate that the test case data had been reviewed by technical staff (TOP-018, para. 6.3 and 6.3.1).
4. No objective evidence could be found to indicate that the procedure-required list of authorized users had been generated (TOP-018, Appendix C and 8.1.3).
5. No objective evidence could be found to indicate that any copies of these programs have been officially released to any user (TOP-018, Appendix C).
6. There is evidence (personnel conversations) to indicate that there are other versions of this software in existence (TOP-018, Appendix C).
7. Objective evidence indicates that TWITCH3 was used in the generation of data for CNWRA 92-019. TWITCH6 is the version currently under CM control (TOP-018, para. 6.2.2.2).
8. No objective evidence exists to indicate what version of MARIANA was used for CNWRA 92-019 (TOP-018, para 6.2.2.2).
9. Software Summary Form for TWITCH does not have a version number associated or stated (TOP-018, para. 5.4).

Initiated by:

Dean Malabro

Date:

2/7/94

PART 2: PROPOSED DISPOSITION AND CORRECTIVE ACTION

Disposition:

accept as is.

Responsible: *P. Nair*
Response Due: *2/8/94*

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2/9/94

Basis of Disposition:

See attached memo.

Action to correct nonconformance:

See attached memo.

Target date for completion: *2.28.94*

Proposed by:

Peter Lichtner

Date:

2.18.94

PART 3: APPROVAL

Element Manager:

[Signature]

Date:

2/18/94

Director of QA:

Dean Malabro

Date:

2/18/94

Comments/Instructions:

PART 4: CLOSE OUT

Comments:

Documentation was reviewed to confirm that the required actions were taken.

Verified by:

[Signature]

Date:

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

Feb. 18, 1994

To: Bruce Mabrito

From: P. Lichtner

PCL

Subject: CNWRA Nonconformance Report No. 94-03, Twitch/Mariana Software Code.

CNWRA NCR 94-03 lists nine discrepancies associated with the current configured Twitch/Mariana software code. I am currently rewriting this code to improve its maintainability, reliability, and portability. In light of my updating efforts, which would render the current configured version obsolete, it would not be cost effective to devote excessive time and money to clear a nonconformance on code that will not be used in the CDM development at the CNWRA. I recommend the following solutions to NCR 94-03:

1. INEL listings for MARIANA state that it is Version 2.0 while Software Summary Form states it is Version 1.0 (TOP-018, para. 5.4).

Enclosure 1, which is a copy of the program currently under CM at INEL identifies the version as Version 1. Based on the evidence, the configured version is Version 1.

2. No objective evidence that the software tools PREFOR, FORWARN, CRAFT, and PCMetrics had been executed (TOP-018, para. 6.3.1).

At the time Twitch/Mariana was placed under configuration management TOP-018 Rev. 0 did not require the evaluation tools to be used, and accounts for this and other nonconformances.

Para. 6.3.1 requires the use of these tools, but in light of the updating effort, I recommend the current configured version of the code not be subjected to the evaluation tools just to clear the NCR. These software evaluation tools will be run on the updated version when it is submitted for CM.

3. No objective evidence found to indicate that the test case data had been reviewed by technical staff (TOP-018, para. 6.3 and 6.3.1).

This item does not exist unless the software evaluation tools noted in item 2 above have been used on Twitch/Mariana; therefore this item does not appear to be a discrepancy.

4. No objective evidence could be found to indicate that the procedure-required list of authorized users had been generated (TOP-018, Appendix C and 8.1.3).

An authorized users list will be generated.

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5. No objective evidence could be found to indicate that any copies of these programs have been officially released to any user (TOP-018, Appendix C).

This code has not been used for its stated purpose (License review process) since placement under CM; therefore no official release should be in evidence.

6. There is evidence (personnel conversations) to indicate that there are other versions of this software in existence (TOP-018, Appendix C).

There are indeed other version of the Twitch/Mariana software package in existence. The other versions are used at the CNWRA as development tools in the current effort to update and improve the software code.

7. Objective evidence indicates that TWITCH3 was used in the generation of data for CNWRA 92-019. TWITCH6 is the version currently under CM control (TOP-018, para. 6.2.2.2).

TWITCH3 will be placed under CM to support CNWRA 92-019.

8. No objective evidence exists to indicate what version of MANANA was used for CNWRA 92-019 (TOP-018, para 6.2.2.2).

The current configured version of MANANA was used in the CNWRA 92-019.
See attached output information.

9. Software Summary Form for TWITCH does not have a version number associated or stated (TOP-018, para. 5.4).

A new Software Summary Form will be issued identifying TWITCH3 as the configured version.



Prasad Nair, EBS Element Manager

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h24594
s 00543/00000/00000
d D 1.1 93/08/04 11:46:32 mmv 1 0
c TWITCH and MARIANA files as composed by John Walton of UT El Paso. This is the original version meant to operate on SUN computer systems. Run times are LONG!
c Placed under VCS by Mark Muller for SWRI CNWRA.

e
u
u
t
t
I 1
c

Subroutine Mariana(xi,ntrial,iwork)
implicit real*8 (a-h,o-z)

c
c Program for simple equilibrium with stoichiometric Gibbs free energy minimization.

Mariana Version 1.0
John C. Walton
8/20/92

134.20.1.1 10:57:18

c
c 8/20/92

include 'param.f'
include 'eq.f'
PARAMETER (NP=maxR)
parameter (tiny = 1.e-8)
DIMENSION ALPHA(maxR,maxR), BETA(maxR), INDX(maxR),
1 xiold(maxR), beta2(maxR), alpha2(maxR,maxR)
dimension xi(maxR)
logical on

c
c A few variable definitions to jog the memory

c
c
c isolv(maxR) = flag for reactions to be solved in a particular iteration
c alpha, alpha2 = second derivative array
c beta, beta2 = first derivative arrays
c ntrial = maximum number of iterations
c iwork = 1 if it converged
c u0 = standard Gibbs Free energy for species i
c iphase = phase for i, 1=aqueous, 2=solid, 3=gas, 4=water
c smass = moles of species per kilogram of water

134.20.1.1 10:57:39

c
c smass = moles of species per kilogram of water
c sact = activity of species i
c xi = reaction progress variable for reaction j
c nspec = number of species
c nreact = number of reactions
c sto = stoichiometric coefficient matrix
c sto(ispec,jreact), negative for reactants, positive for products
c maxS, maxR = maximum number of species and reactions
c xiold = the old value of xi

ENC 1