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SOFTWARE RELEASE NOTICE

01. SRN Number: GHGC-SRN-144		
02. Project Title: SIMUL Version 1.0		Project No. 20-5708-561
03. SRN Title: SIMUL Version 1.0		
04. Originator/Requestor: Bruce Mabrito		Date: 05/09/97
05. Summary of Actions <ul style="list-style-type: none"> <input checked="" type="checkbox"/> Release of new software—This is software that R. Pabalan obtained from a colleague and intends to utilize. <input type="checkbox"/> Release of modified software: <ul style="list-style-type: none"> <input type="checkbox"/> Enhancements made <input type="checkbox"/> Corrections made <input type="checkbox"/> Change of access software <input checked="" type="checkbox"/> Software Retirement <div style="text-align: right; margin-top: 10px;"> <i>E.C. Ruz</i> 12/5/2001 </div>		
06. Persons Authorized Access		
Name	RO/RW	A/C/D
Roberto Pabalan		Addition
07. Element Manager Approval: <i>E.C. Ruz</i>		Date: <i>5/12/97</i>
08. Remarks: <p style="text-align: center;">Acquired software, not to be modified</p>		

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SOFTWARE SUMMARY FORM

01. Summary Date: 05/09/97	02. Summary prepared by (Name and phone) Roberto Pabalan, (210) 522-5304	03. Summary Action: New	
04. Software Date: 01/02/95	05. Short Title: SIMUL Version 1.0		
06. Software Title: SIMUL Version 1.0		07. Internal Software ID:	
08. Software Type: <input type="checkbox"/> Automated Data System <input checked="" type="checkbox"/> Computer Program <input type="checkbox"/> Subroutine/Module	09. Processing Mode: <input type="checkbox"/> Interactive <input type="checkbox"/> Batch <input checked="" type="checkbox"/> Combination	10. APPLICATION AREA a. General: <input type="checkbox"/> Scientific/Engineering <input checked="" type="checkbox"/> Auxiliary Analyses <input type="checkbox"/> Total System PA <input type="checkbox"/> Subsystem PA <input type="checkbox"/> Other b. Specific: Cement/Water Interaction	
11. Submitting Organization and Address: CNWRA 6220 Culebra Rd. San Antonio, TX 78228		12. Technical Contact(s) and Phone: Roberto Pabalan, (210) 522-5304	
13. Narrative: Chemical modeling program for cement/water interaction			
14. Computer Platform IBM Compatible	15. Computer Operating System: MS DOS	16. Programming Language(s): Fortran 77	17. Number of Source Program Statements: 925
18. Computer Memory Requirements: 8 MB	19. Tape Drives:	20. Disk/Drum Units:	21. Graphics:
22. Other Operational Requirements			
23. Software Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY		24. Documentation Availability: <input type="checkbox"/> Available <input checked="" type="checkbox"/> Inadequate <input type="checkbox"/> In-House ONLY	
Software Custodian: <u></u>		Date: <u>5/9/97</u>	

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

SOFTWARE CONTROL CHECKLIST

Name of Software: SIMUL

Version: 1.0

Primary User: Roberto Pabalan

- SOFTWARE REQUIREMENTS DESCRIPTION
 - Documentation

- DESIGN AND DEVELOPMENT
 - Documentation (Scientific Notebook)

- DESIGN VERIFICATION
 - Computer runs uniquely identified
 - Software analysis tools have been applied and discrepancies resolved
 - Design Verification Report

- INSTALLATION TESTING
 - Installation test documentation—Scientific Notebook #185, Vol. 1, pages 8-13
 - Discrepancy resolution

- CONFIGURATION CONTROL
 - Software Summary Form
 - User's Manual
 - Technical Description
 - Source Code (not applicable)
 - Version Control (not applicable)
 - Software Release Notice

- SOFTWARE PROBLEM REPORTING AND RESOLUTION
 - Software Problem and Change Request

- SOFTWARE VALIDATION
 - Software Validation Test Plan
 - Software Validation Test Report
 - Software Validation Review

- SOFTWARE RETIREMENT
 - Software Release Notice

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To: Bruce Mabrito at CNWRA-OS2
From: Roberto Pabalan
Receipt Requested
Subject: SIMUL code installation and testing documentation
03-17-97 09:59 AM

TO: Bruce Mabrito
Director of QA

FROM: Roberto Pabalan
Senior Res. Scientist

Subject: Documentation for installation and testing of the SIMUL code

For the record, the installation and testing of the SIMUL code for simulating cement/water interactions was documented in laboratory notebook #185, Volume 1, pages 8-13. Additional verification calculations are described in electronic notebook #185, Volume 2, pages 1-14.

To: Bruce Mabrito at CNWRA-OS2
CC: English Percy
From: Roberto Pabalan
Receipt Requested
Subject: SIMUL code
02-28-97 03:29 PM

MEMORANDUM

February 28, 1997

TO: Bruce Mabrito, QA Director

FROM: Roberto Pabalan, Senior Research Scientist

SUBJECT: SIMUL - A chemical equilibrium code for cement/water interactions

SIMUL was and is being used for scoping calculations of cement/water interactions relevant to understanding the geochemistry of the near-field environment (ENFE KTI). The subject code was acquired through John Westall, University of Oregon. The code was developed by Eric Reardon (University of Waterloo) based on his thermodynamic model which was described in the publication "Problems and Approaches to the Prediction of the Chemical Composition in Cement/Water Systems" (Waste Management vol. 12, pp. 221-239, 1992). A copy of this paper will be sent to you shortly. A copy of the program, including sample input and output files, were provided to you earlier subsequent to publication of the 1996 CNWRA Annual Report.

The code was installed in a Windows 3.1 compatible machine. Test calculations were done and comparisons with literature data were documented in Scientific Notebook vol. 185. No changes to the code are planned at present.

Let me know if you need additional information.

Information on Pages 6 through 24 contains Problems and Approaches to the Prediction of the Chemical Composition in Cement/Water Systems copyright information and is therefore not included in this file.