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SOFTWARE RELEASE NOTICE

01. SRN Number: RDCO-SRN-122

02. Project Title:
Thermal Effects on Flow

Project No.
20-5708-661

03. SRN Title: CTOUGH 1.0 (SUN)

04. Originator/Requestor: Robert Brient RB

Date: 02/02/96

05. Summary of Actions

■ Release of new software

□ Release of modified software:

□ Enhancements made

□ Corrections made

□ Change of access software

☑ Software Retirement Attc 11-26-01

06. Persons Authorized Access

Name	RO/RW	A/C/D
R. Green P. Lichtner		

07. Element Manager Approval:

Date: 2/8/96

08. Remarks:

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SOFTWARE SUMMARY FORM

01. Summary Date: 01/30/96

02. Summary prepared by (Name and phone) R.D. Brient, 522-5537

03. Summary Action: New

04. Software Date: 08/15/93

05. Short Title: CTOUGH Version 1.0

06. Software Title:

CTOUGH - Thermal and Hydrologic Simulation of Large-Scale Problems in Nuclear Waste Isolation.

07. Internal Software ID: NONE

08. Software Type:

□ Automated Data System

■ Computer Program

□ Subroutine/Module

09. Processing Mode:

□ Interactive

□ Batch

■ Combination

10. APPLICATION AREA

a. General:

■ Scientific/Engineering □ Auxiliary Analyses

□ Total System PA

□ Subsystem PA □ Other

b. Specific:

11. Submitting Organization and Address:

CNWRA, SwRI, San Antonio, Texas

12. Technical Contact(s) and Phone:

Ron Green, (210) 522-5305

13. Narrative:

CTOUGH - CTOUGH is used to numerically simulate the thermal and hydrologic environment around nuclear waste packages in the unsaturated zone for the Yucca Mountain Project.

14. Computer Platform: SUN

15. Computer Operating System: UNIX

16. Programming Language(s): FORTRAN

17. Number of Source Program Statements: 15,845 lines of code

18. Computer Memory Requirements: UNKNOWN

19. Tape Drives: NONE

20. Disk/Drum Units: N/A

21. Graphics: UNKNOWN

22. Other Operational Requirements

NONE

23. Software Availability:

■ Available □ Limited □ In-House ONLY

24. Documentation Availability:

■ Available □ Inadequate □ In-House ONLY

Software Custodian: RDBrient Date: 2/8/96

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

SOFTWARE CONTROL CHECKLIST

Name of Software: CTOUGH Version: 1.0

Primary User: Ron Green KTI - Thermal Effects on Flow, 20-5708-661
CTOUGH was modified from VTOUGH by the CNWRA before 3/95.

□ 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 #150, Pg 107-108 ☒

Discrepancy resolution □

☒ CONFIGURATION CONTROL

Software Summary Form ☒

User's Manual: TOUGH User's Guide, 6/87 (LBL)*, Draft V-TOUGH - An Enhanced Version of the TOUGH Code for the Thermal and Hydrologic Simulation of Large-Scale Problems in Nuclear Waste Isolation 11/89 (LLNL)*. CNWRA Report 94-026, 10/1994. ☒

Technical Description: TOUGH User's Guide, 6/87 (LBL)*, Draft V-TOUGH - An Enhanced Version of the TOUGH Code for the Thermal and Hydrologic Simulation of Large-Scale Problems in Nuclear Waste Isolation 11/89 (LLNL)*. CNWRA Report 94-026, 10/1994. ☒

*Located in QA Records Package QAR305 Q199403310002.

Source Code: CTOUGH version 1.0, 1/29/96 ☒

Version Control ☒

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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MEMORANDUM

To: Bob Brient

From: George Rice GR

Date: March 8, 1996

Subject: Installation testing of CTOUGH

I have completed the installation testing of CTOUGH as required by TOP-018. A CTOUGH simulation was performed on Sneezy (CNWRA 305). The results were reasonable and comparable to results obtained by other workers that have simulated similar problems. This testing is documented in CNWRA notebook 150, pages 107 and 108.

Installation test for CTOUGH

Scientific Notebook #150 pg 107-108

CTOUGH 1.0

CNWRA 94-026 5/15

ENGINEERED BARRIER SYSTEM PERFORMANCE ASSESSMENT CODES (EBSPAC) PROGRESS REPORT OCTOBER 1, 1993, THROUGH SEPTEMBER 25, 1994

Prepared for

Nuclear Regulatory Commission
Contract NRC-02-93-005

Prepared by

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

October 1994

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2 NEAR-FIELD ENVIRONMENT MODEL

2.1 INTRODUCTION AND RATIONALE

To support near-field modeling efforts, it was deemed necessary to upgrade the two-phase fluid flow code VTOUGH (Nitao, 1989) currently in use at the CNWRA. The current version of VTOUGH installed at the CNWRA was inefficient to use in several aspects and did not compute all the requisite quantities needed for evaluating the near-field performance of a high-level nuclear waste (HLW) repository emplaced above the water table in unsaturated porous media. These aspects include the evaporation rate and relative humidity. The VTOUGH input file was rigidly formatted making it cumbersome to alter without causing error. Output from the VTOUGH code was captured from a screen dump and processed with a post-processor. This resulted in a large output file with wasted disk space and inefficient monitoring of the progress of the execution of the code. To correct the deficiencies in the original code, a free-format input file was developed, and output files for plotting were written at user-specified times. More efficient solvers were added to the code, including an efficient direct solver which reduced the amount of computer memory required as well as the computational time.

2.2 MODIFICATIONS TO THE VTOUGH CODE

Specifically, modifications to the VTOUGH code included:

- I/O
  - — Free-format input
  - — Output plot files created at user-specified times
  - — Time-history plot files
- Solvers
  - — Nonsymmetric Preconditioned Conjugate Gradient (NSPCG) package
  - — Nested factorization
  - — D4 direct solver
- Evaporation Rate Computation
- Relative Humidity Computation

There are about 15 available preconditioners and about an equal number of accelerators available in the NSPCG package, giving 225 different combinations. Comparing the various solvers is still ongoing. The most successful solver to date is the D4 solver which increases CPU time by a factor of 2.5 or more and reduces storage by a factor of 3 or more. As a consequence, much larger systems can be computed than were previously possible without increasing workstation memory requirements.

2.3 DESCRIPTION OF CTOUGH

The code VTOUGH (Nitao, 1989) solves the two-phase mass and energy conservation equations in a partially saturated porous medium with components water and air. CTOUGH is based on the VTOUGH requirements and is modified to provide more user-friendly I/O and reduce computer computation time and memory. It was found that computation time could be reduced by at least a factor of 2.5 and memory by a factor of 3.5 or more, depending on the problem. This enables larger problems to be run with finer grids in two or three spatial dimensions.

The CTOUGH could be used in future work to analyze moisture redistribution in the near-field region of a HLW repository resulting from the thermal perturbation caused by emplacement of the waste. CTOUGH may also be combined with the electromigration code GEM to analyze salinity buildup around waste packages due to reflux of liquid and evaporation/condensation effects. Currently, CTOUGH is being used to analyze the release of ^{14}C from the repository by providing a spatial and temporal description of the temperature field, saturation, and liquid and gas fluxes resulting from emplacement of HLW.

This section provides a brief introduction to running the CTOUGH code and the input file conversion program that converts from the old formatted input file to the new free-format version. Modifications to the input file and structure of the output files for plotting are presented in Appendix A.

2.3.1 Execution of CTOUGH

The computer program CTOUGH is executed by invoking the following command on a UNIX machine in a shell window:

```
ctough data        (for an interactive run)

ctough data &      (for a batch or background run)
```

where ctough is the name of the CTOUGH executable module, and 'datai' is the name of the input file. Note that all data file names must end with the character '*i*', and should not exceed seven characters. The last character '*i*' of the data file name should not be specified on the command line as shown above.

If a data file name is not specified, the default dataset named '*toughi*' will be used. If the specified or default data file does not exist in the current directory, the run is terminated. The system will ask the user to re-specify the dataset name for an interactive job and terminate if running in batch mode.

The output files are identified by the dataset name prefix as discussed in Appendix A. Thus, a number of jobs may be concurrently submitted which will produce different output files corresponding to different dataset names.

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2.3.2 Execution of Conversion Program

To enable easy conversion from existing input files using the original version of VTOUGH, a conversion program was constructed to facilitate converting to the free-format input file used by CTOUGH. To execute the conversion program the user types:

```
convrt < dataold > datai
```

where convrt is the executable of the conversion program, dataold is the input file corresponding to the old fixed format, and datai is the converted new file compatible with the free-format modified CTOUGH.

Currently, the CTOUGH code is in the development and evaluation stage. A user's manual is planned to be issued in FY96 and will be followed by inclusion of the code in the software configuration management process at the CNWRA.

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CTOUGH INPUT/OUTPUT MODIFICATIONS

A.1 INPUT FILE SPECIFICATIONS

Element data corresponding to the keywords 'ELEME' and 'CONNE' must be read in the order of increasing row number. That is, read column-by-column with increasing depth. The elements, if not read in the above order, will result in improper calculations of coordinates of elements used in plotting. Also, this order is required for conjugate gradient methods. An example is given below to illustrate the data structure.

Example:

```
ELEME
A     1     matr1     1.e+3
A     2     matr1     1.e+3
A     3     matr3     1.e+3
.     .     .         .
A     15    matr1     1.e+4
B     1     matr1     1.e+3
B     2     matr1     1.e+3
B     3     matr3     1.e+3
B     .     .         .
B     15    matr1     1.e+4
C     1     matr1     1.e+3
C     2     matr1     1.e+3
.     .     .         .
.     .     .         .

   CONNE
   A    1    B    1    ....
   A    2    B    2    ....
   A    3    B    3    ....
   .    .    .    .    ....
   A    15   B    15   ....
   B    1    C    1    ....
   B    2    C    2    ....
   .    .    .    .    ....
   B    15   C    15   ....
   .    .    .    .    ....
   .    .    .    .    ....
   A    1    A    2    ....
   A    2    A    3    ....
   .    .    .    .    ....
```

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A.1.1 Solution Method

The program will use, by default, the Band matrix solver. For all other solvers, the solution method must be specified. It is best to specify the solution method in the input-data, even for the default method. This is done with the keyword SOLVER.

A.1.2 Evaporation Element Specification

If the cumulative evaporation is to be written for each time step for specified elements, data for such elements must be specified by a keyword 'EVAP' followed by element names, and the read sequence must be terminated by reading the last element with zeros or blank. The evaporation rate will be computed for all the elements and printed at the specified times along with the other state variables, irrespective of reading this dataset. In the absence of this keyword, no output will be written on unit dataEVP.xyp (see Section A.2). If rates are to be computed, derivatives of the cumulative evaporation with respect to time can be easily calculated, as the cumulative time is also available in this file.

Example:

```
EVAP
A   3
A   4
B   3
B   4
A   :blank line
```

Coordinate Calculations: Coordinates for each element identify the center of the block element with the origin placed at the bottom of the first column. In the above example, the element A 15 will be placed at the origin. It is assumed that all problems are 2D, and as such, the y-coordinate is designated to be zero for all elements.

A.1.3 Utility Keywords

The input data deck may contain certain utility-keywords, the use of which is optional. They are briefly outlined below.

1. Read - : comments

comments = Any comments or information the user wishes to enter including all blanks starting from column 2 through 80 inclusive. Comment cards are ignored by the simulator and used simply to clarify or introduce notes on any desired data. They can also be used for putting titles or headings on input variables, etc.

Example : ——

```
:Relative permeability of water is changed
:By a factor of 1.5
```

2. Read - IECHO

IECHO = LIST if input data images are to be printed.

= NOLIST if input data images are not to be printed.

Default value of IECHO = NOLIST

The input-data list will be written on file *.ERRS. If a partial list of input data is desired, insert a NOLIST card after which printing of the list is to be suppressed, and a LIST card from which printing is to be resumed. Repeated use of LIST and NOLIST cards will enable printing the desired sections of the total input data stream. LIST or NOLIST cards themselves will not be printed in the card images. Irrespective of IECHO options, a message giving the total number of cards read is printed prior to execution of the run.

Example:

```
|
|
Data              Print card images
|
|
       NOLIST
|
|
Data              Suppress card images
|
|
       LIST
|
|
Data              Print card images
|
|
       NOLIST
|
|
Data              Suppress card images
|
|
```

3. Read - NCOL (N)

NCOL = Keyword indicating that this is the NCOL card, simply enter NCOL

N = Number of columns from column 1 to N inclusive, which will be read on subsequent data cards. This is refered to as the 'active field' of a card or line. The user may enter any comments or information beyond the active field which will be listed but not processed. The default value of N=80 is used. N must not be greater than 80. Repeated use of a NCOL card with different values of N will have the effect of widening or narrowing the width of the active field.

Example:

```
                    NCOL 60

         |
         |
         Data       Active field of 60 characters
         |
                    NCOL 80
         |
         |
         Data       Active field of 80 characters

         |
         |
                    NCOL 70
         |
         Data       Active field of 70 characters
         |
```

4. Read - ISKIP

ISKIP = SKIP if input data is to be skipped and not processed until a NOSKIP card is encountered.

= NOSKIP if input data following this card is to be processed. This card has no effect if a SKIP card is not introduced prior to this card. It, in effect, negates the effect of a SKIP card.

If a segment or block(s) of data is not to be processed, insert a SKIP card at the beginning of such block and enter a NOSKIP card at the bottom of the block. Repeated use of SKIP and NOSKIP cards will have the effect of removing the data between SKIP and NOSKIP in the data deck during execution while preserving the entire input data intact. If a NOSKIP card is not encountered following a SKIP card, all the data from SKIP will be removed. Irrespective of LIST or NOLIST options invoked, data between SKIP and NOSKIP cards will not be echoed or listed.

Example:

```
          |
          |
          Data
          |
          |
          SKIP
          |
          |
          Data        Remove this data beginning
                      with SKIP until NOSKIP
                      card is encountered
          |
          |
          NOSKIP
          |
          |
          Data        Process this data beginning
                      after NOSKIP
          |
          |
```

A.2 OUTPUT FILES

Output is directed to several different files as tabulated below. Note that the file names are associated with the input data file name as prefix.

File Names	Unit #	Description
data.OUT	6	Output of VTOUGH including contents of unit 66 and 67 described below
data.HIS	8	Time history information for post-processing purposes
dataTMP.xyp	25	Temperature time-history at designated elements
dataTCP.xyp	30	Temperature and capillary pressure time-history at designated elements
dataSAT.xyp	35	Saturation time-history at designated elements
data.SAVE	60	Initial condition data for subsequent runs
data.BAL	61	Incremental and cumulative energy balance for each time step
data.COEF	62	Flow and accumulation coefficients: written only if specified by input data directives

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File Names	Unit #	Description
data.ERRS	63	All error messages and requested input data images
dataEVP.xyp	64	Cumulative evaporation for designated elements, for every time step
dataVELn.xyp	65	Velocity of fluids for specified time steps
dataVARn.xyp	66	Field variables including condensation rate for all elements at specified times
data.PCT	67	Capillary pressure curve depicting height versus saturation
data.MESH	3	Mesh or element file (scratch)
data.CON	4	Element connection file (scratch)
data.GEN	16	Sink/source generation file (scratch)