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User Information Document for: TOUGH2 V1.11MEOS9NT V2.0

REV. NO.: 00E

Document ID: 10065-UID-1.11MEOS9NTV2.0-01

STN: 10065-1.11MEOS9NTV2.0-01

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REVISION HISTORY

<u>Revision</u>	<u>Date</u>	<u>Purpose of the Revision</u>
00A	12/27/2006	Initial issue
00B	12/28/2006	Revised per comments
00C	12/29/2006	Updated Figure 1
00D	2/4/2007	Revised per IV&V review
00E	4/1/2007	Corrected acceptance criteria per IV&V comment

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1. INTRODUCTION

1.1 PURPOSE

The objective of the User Information Document is to provide information to the end-user on how to effectively install and use the software referenced on the title page.

1.2 SOFTWARE IDENTIFICATION

This document contains the user information of the software identified on the title page.

The Software Configuration Control Request (SCCR) (Software Tracking Number [STN]: 10065-1.11MEOS9NTV2.0-01) specifies the plan used to produce this document.

Requirement Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-RD-1.11MEOS9NTV2.0-01) specifies the requirements that the design implements.

Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01) specifies the design and validation test cases.

1.3 DEFINITIONS

- **Dynamic Memory Allocation** is the allocation of memory storage for use in a computer program during the runtime of that program. It is a way of distributing ownership of limited memory resources among many pieces of data and code. A dynamically allocated object remains allocated until it is deallocated explicitly.

1.4 TRACEABILITY

The Requirement Traceability Matrix (Document ID: 10065-RTM-1.11MEOS9NTV2.0-01) documents the relationships between the following:

- The Requirements (as specified in the RD) and the design elements (as specified in the DD)
- The Requirements (as specified in the RD) and the validation test cases (as specified in the DD)
- The User Information Document (as specified in section 2) and requirements (as specified in the RD).

2. USER INFORMATION

2.1 INTRODUCTION

This software is to be used for radionuclide transport studies in the subsurface. We describe all the necessary steps and activities to install the software, test the installation, and confirm the results of the installation test. This software cannot be used under non-isothermal conditions.

2.2 HOW TO USE THIS SOFTWARE

This software is designed to be used in a UNIX environment. The software is to be installed as instructed below (see Section 3) and the compiled executable, EOS9nT, can be copied to user's working folder and run by designating input and output files.

2.3 INTERACTIONS WITH THE SOFTWARE

There are no user interactions during the execution.

2.4 REQUIRED TRAINING

The users must be trained to be familiar with (1) solute and colloid transport and (2) the specifications of input and output files provided in Attachments of Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01).

2.5 INPUT SPECIFICATION

Input specifications are described in Attachment A in Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01).

2.6 OUTPUT SPECIFICATION

The concentration output is in terms of mass fraction, thus its range is between 0 and 1. Output Data and Output specifications generated by the code are available in Attachment B in Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01).

2.7 DATA FILES

The input data files are described in Attachment A. Output data files are described in Attachment B in Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01).

2.8 DEFAULTS

A number of default values are available in Attachment A of Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01).

2.9 ERRORS

For a description of error and user responses, see Attachment B.

2.10 HARDWARE/SOFTWARE ENVIRONMENTS

This software is run on a UNIX workstation. There are no external software systems or database managers associated with this software other than the operating system and a FORTRAN 90 compiler.

Table 2.10.1 Hardware/Software environments

Hardware	Software
Alpha Computer System	OSF1 V4.0 with Digital Fortran 90 V5.2; or OSF1 V5.1 with Compaq Fortran 90 V5.4

2.11 SAMPLES

No Sample tests are being provided.

3. INSTALLATION AND VALIDATION

3.1 INSTALLATION AND INSTALLATION VERIFICATION

3.1.1 Pre-Installation Activities

Verify that the target computer system meets the system requirements in Section 2, and that 500 MB of disk space is available.

3.1.2 Installation Instruction and test process

Table 3.1.2.1 Installation instruction and result

Step	Installation Activity	Expected results
1. Transfer	<p>Copy the eos9nt20.tar.gz archived file from the distribution media to a directory on a unix alpha system with OSF1 V4.0/5.1. Transfer this file in a binary mode.</p> <p>Go to this directory and unpack the archive, e.g.:</p> <pre>gunzip eos9nt20.tar.gz tar -xvf eos9nt20.tar</pre>	<p>The file will be decompressed in the working directory. A new directory is created namely "EOS9nTV20". The decompressed file EOS9nTv2.0_Code contains two directories: EOS9nTv2.0_Code and TestProblems inside the parent directory EOS9nTV20.</p> <p>The TestProblems directory contains an installation test folder InsTest and six test folders: Test#1_F, Test#2_F, Test#3_F, Test#4_F, Test#5_F, Test#6_F.</p>
2. Compiling, linking and building	<p>"cd" to the SourceCode directory and compile the code:</p> <pre>cd EOS9nTV20/EOS9nTv2.0_Code make</pre>	<p>The executable module T2E9nTx is built by the compilation process.</p>

3.1.3 Post-Installation Activities

Retain all the directories of the installed software system in order to perform the Validation Test Process.

Delete the directory EOS9nTV20 (e.g., `rm -IR EOS9nTV20`. This command must be executed from a directory context that does not contain the directory to be removed.).

3.1.4 Installation Validation

There is one installation validation test case provided with this software. The installation test case 1(IT-01) is listed in the table below (table 3.1.4.1).

Table 3.1.4.1 Installations steps and results

Step	Installation Activity	Expected results
1. Changing directory	“cd” to the installation test directory cd ../TestProblems/InsTest F	Directory changed.
2. Execution	Run T2E9nTx from the command line, designating “InsTest.out” as the output name (see attachment for detailed description). ../EOS9nTv2.0_Code/T2E9nTx < InsTest >InsTest.out	No execution error occurs.
3. Comparison	Compare “InsTest.out” to the reference output file “InsTest.outR.out” .	The file comparison meets the acceptance criteria described below in this section

If the comparison of the results of the installation test output file “InsTest.out” and those in the reference output file InsTest.outR” provided in the installation media shows that

- (a) Using an initial reference mass fraction of 1, when the mass fraction in "InsTest.out" and "InsTest.outR" are larger than $1.0e-6$, the mass fractions in "InsTest.out" and "InsTest.outR.out" differ less than 5%, or
- (b) the mass balances of the tracers differ by less than 5%,

(whichever is larger), then the installation test is passed, installation is complete, and the code is ready for application.

Upon completion of each test, the test results of the output file InsTest and the reference output file InsTest.outR.out shall be recorded in the Log of Test Results (Attachment C)

3.2 VALIDATION TESTS

Validation test cases for EOS9nT V2.0 are provided as Attachment D. Upon completion of each test, the test results shall be recorded in the Log of Test Results (Attachment E).

The difference between the mass balance and mass fraction in the new runs and the output provided with the media should be less than 5% to pass the acceptance.

The spreadsheets of all the validation test result are located in the media, namely TestValiation1-5.xls and TestValiation6.txt

3.3 CONTINUOUS USE SOFTWARE

This software is not intended for continuous use. It is meant to be run as needed to simulate the transport of tracers (solutes or colloids) at the Yucca Mountain.

4. REFERENCES/ATTACHMENTS

4.1 REFERENCE

Software Configuration Control Request for TOUGH2 V1.11MEOS9NT V2.0. (Software Tracking Number: 10065-1.11MEOS9NTV2.0-01)

Requirement Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-RD-1.11MEOS9NTV2.0-01.

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IT-PRO-0012, Rev.1., Qualification of Software. DOC.20060929.0006

IT-PRO-0013, Rev.1., Software Independent Verification and Validation. DOC.20060929.0019

4.2 ATTACHEMENTS

A. Input Data Files

B. Warnings and Error Handling Requirements

C. Installation Test Log

D. Validation Test Cases

E. Validation Test Log

ATTACHMENT A INPUT DATA FILES

A.1 Input Data Blocks

The following table is the description of what the input data blocks are to be for the software. Input Data Requirements and Specifications are located in Attachment A in Design Document.

Table A.1.1 Input data blocks

<i>Data Block</i>	<i>General Description</i>
ALLOC	Dynamic Memory Allocation Parameters
ROCKS	Rock Properties
PARAM	Simulation Parameters
ELEME	Gridblock Geometry
CONNE	Gridblock Connections
TRACR	Tracer Information
INCON	General Initial Conditions
INDOM	Domain-specific Initial Conditions
GENER	Source and Sink Information

These files will follow the formats established by Pruess (1991).

A.2 Input Requirements

ALLOC

1. This block must always be placed at the beginning of the input data file because there is no a priori array dimensioning.

ROCKS

1. Adjust porosity and tortuosity of top grid blocks to prevent non-physical behavior of tracers diffusion through them.
2. Add immobile water saturation, longitudinal and transverse dispersivity, transfer coefficient between mobile and immobile water phases, and bulk porosity of fracture.
3. Use fictitious rock domain to provide reference conditions.
4. Apply multipliers to relative permeabilities and capillary pressures.

PARAM

1. Identify number of tracers to be considered
2. Flag read/write of UNVEC file containing unit vectors normal to gridblock interfaces.
3. Flag read/write of VELOC file containing water flux, pore velocity, Darcy velocity, interface area and upstream weighting factor at each connection.
4. Flag read of INCON and START initial conditions containing default initial mass fractions of tracers in the water, initial primary component of the sorbed or filtered mass, and initial secondary component of the sorbed or filtered mass.

ELEM

1. Add information to determine unit vectors at the centers of the two elements across each

connection for the dispersion tensor calculation.

CONNE

Introduces information for the connections (interfaces) between elements. It follows requirements and specification of conventional TOUGH2.

TRACR

1. Add parameters to define:
 - NTRACR: number of tracers
 - MXTRDT: maximum number of timesteps
 - NOITTR: maximum number of Newton iterations
 - FLOWFI: steady-state of transient flow field for transport
 - LPLACE: whether to use Laplace transform formulation for transport
 - NITR: number of summation terms for inversion of the Laplace space solution
 - CRLAPL: convergence criteria for conjugent gradient solver of Laplace matrix
 - NOPRNP: flag to print mass and volume balances of phases and tracers
2. Add parameters to define:
 - IFFACT: indicator for flow velocity averaging
 - ISFACT: indicator for water saturation averaging
 - IDFACT: indicator for radioactive decay averaging
 - ICOVRD: indicator for overriding default Courant number
 - ITOVRD: indicator for overriding default half-life
 - COURAN: maximum allowable Courant number
 - HLFAC: maximum allowable tracer half-life
3. Tracer Information
 - TRACER: tracer name
 - TRTYPE: tracer type
 - PCTYPE: tracer decay type
 - NMROCK: number of sorption domain coefficients
 - IDROCK: default sorption domain coefficients
 - NDAUTR: number of daughter products
 - NADDID: additive group index daughter decay products
 - IDPARE: parent identifier
 - IDSEQ: decay sequence number for daughter
 - MATCOL: rock number of colloid
 - DD00: molecular diffusion coefficient
 - HAFLIF: tracer half life
 - WTMOL: molecular weight of the tracer
 - ZETA: decay mass fraction of sorbed parent that remains sorbed as daughter
 - RHOCOL: colloid density
4. Sorption Information
 - NNROCK: sequence number of the rock domain
 - NSORTP: flag for tracer sorption type
 - NOSAME: additional rock information
 - DDSS: tracer surface diffusion coefficient

- SKD: tracer sorption information
- 5. Colloid Information
 - ALPHCL: longitudinal dispersivity
 - ALPHCT: transverse dispersivity
 - COVLFA: velocity adjustment factor
 - COLEFF: single collector efficiency
 - ENTRFR: accessibility factor
 - COLDIA: colloid diameter
 - PORDIA: grain diameter or fracture aperture
 - PERKIM: kinetic reverse filtration coefficient

INCON

Add number of tracers for initialization, their mass fractions, primary sorbed or filtered concentrations, and secondary sorbed or filtered concentrations.

INDOM

Number of colloids for initialization, their mass fractions, primary sorbed or filtered concentrations, and secondary sorbed or filtered concentrations.

GENER

Add mass fraction of tracer (solute or colloid) in the injected phase.

ATTACHMENT B WARNINGS AND ERROR HANDLING REQUIREMENTS

If inputs indicate conflicting conditions and/or parameter values are outside realistic ranges, EOS9nT is to respond according to the severity of the violation. Non-critical conflicts shall result in a warning or clarifying message, internal adjustment of the corresponding conditions and/or parameters, and continuation of the simulation. Serious violations shall result in an error message identifying the problem, and the simulation is to be aborted.

B.1. Warning Messages

Warnings are to be printed, and the corresponding internal adjustments are to be made, in the following cases:

1. The number of rocks/soils for which sorption parameters are provided is larger than the number NM in data block ROCKS. Then only the sorption of the first NM rocks are to be used, and the rest are to be ignored.
2. If a rock/soil porosity $\text{PHI} > 2$ in ROCKS, it represents an 'atmospheric' domain, and its tortuosities and dispersivities are to be reset to 0.
3. A gridblock has no domain assignment. Then the properties of domain 1 are to be assigned to the gridblock.
4. The number of significant digits is between 9 and 12. The message shall warn the user to expect deteriorating convergence behavior.
5. The number of significant digits in double precision arithmetic is equal or less than 8. The message shall warn the user of insufficient significant digits, potential convergence failure, and the need to employ double precision arithmetic.
6. There are no tracers in the system (cc NTRACR=0). Then only the flow equation shall be solved.
7. If ITRACR \neq 0 in PARAM and the data block TRACR is missing, ITRACR is to be reset to 0, and only the flow equation is to be solved.
8. If MXTRDT \leq 0 (see data block TRACR), it is to be reset to 99999 (default).
9. If FLOWFI \neq 'TRANSI' and FLOWFI \neq 'STEADY' (see data block TRACR), FLOWFI is to be reset to 'STEADY' (default).
10. If the flag for the Laplace transform formulation LPLACE $<$ 0 and LPLACE $>$ 1 (see data block TRACR), LPLACE is to be reset to 0 (default) and conventional timestepping is to be employed.
11. If the number of the summation terms in the Stehfest Laplace transform formulation NITR $<$ 10 or NITR $>$ 18 (see data block TRACR), NITR is to be reset to 18.
12. If the number of the summation terms in the DeHoog Laplace transform formulation NITR $<$ 5 or NITR $>$ 10 (see data block TRACR), NITR is to be reset to 6 (default).
13. If the number of the summation terms in the Stehfest Laplace transform formulation NITR is an odd number (see data block TRACR), NITR is to be reset to $\text{min}(\text{NITR}+1, 18)$.

14. If the maximum number of allowable Newtonian iterations in the tracer equations $NOITR \leq 0$ (see data block TRACR), $NOITR$ is to be reset to 5 (default).
15. If the flag for flow velocity averaging $IFFACT < 0$ or $IFFACT > 3$ (see data block TRACR), $IFFACT$ is to be reset to 0 (default).
16. If the flag for water saturation averaging $ISFACT < 0$ or $ISFACT > 3$ (see data block TRACR), $ISFACT$ is to be reset to 0 (default).
17. If the flag for radioactive or reactive decay averaging $IDFACT < 0$ or $IDFACT > 1$ (see data block TRACR), $IDFACT$ is to be reset to 0 (default).
18. If the maximum Courant number $COURAN > 1$ and the flag for overriding it $ICOVRD \neq 9$ (see data block TRACR), $COURAN$ is to be reset to 1 (default). Note that $COURAN = 1$ is necessary for the explicit solution of the tracer equation(s). In EOS9nT, however, the tracer equation(s) are to be solved implicitly. Thus $COURAN = 1$ would impose a very (and unnecessarily) conservative condition, and could be substantially relaxed with impunity.
19. If the maximum allowed time step as a fraction of the half-life or the forward reaction constant $HLFRAC > 0.1$ and the flag for overriding it $ITOVRD \neq 9$ (see data block TRACR), $HLFRAC$ is to be reset to 0.1 (default).
20. If the convergence criterion of the Laplace space solutions $CRLAPL < 1.0E-14$ or $CRLAPL > 1.0E-09$ (see data block TRACR), $CRLAPL$ is to be reset to $1.0E-12$ (default). The strict convergence criterion is necessitated by the need for very accurate Laplace space solutions for accurate time domain solutions.

B.2. Error Messages

Error messages are to be printed, and the simulations are to be aborted, in the following cases:

1. If the number of (a) elements, (b) connections, (c) sinks and sources or (d) the work array elements declared in the main program (module T2CG1.f) are smaller than the needed values (to be determined internally by EOS9nT from the input file).
2. If there is a discrepancy between the array dimensions in the main program (module T2CG1.f) and in the included module TRCOMN.f. This could occur if (a) the numbers of elements, (b) the numbers of connections, (c) the numbers of sink and sources or (d) the numbers of elements in the work arrays differ in the two modules.
3. If the number of tracers $ITRACR$ declared in PARAM (see card 5.2.1) exceeds the maximum tracer number $NTRCMX$ declared in the module TRCOMN.f.
4. If the number of tracers $NTRACR$ declared in data block TRACR exceeds the maximum tracer number $NTRCMX$ declared in the module TRCOMN.f.
5. If the number of tracers $NTRQ$ declared in data block GENER (see card 5.7.1) differs from the number of tracers $NTRACR$ declared in data block TRACR.
6. If the number of tracers $NTRACR$ declared in data block TRACR differs from the number of tracers $ITRACR$ declared in the data block PARAM.
7. If the number of tracers $KTRACR$ declared in data block INCON differs from the number of tracers $NTRACR$ declared in the data block TRACR.

8. If the number of rocks/soils for which sorption/filtration data are provided in data block TRACR exceeds the number of rocks/soils provided in data block ROCKS.
9. If the tracer type TRTYPE and the sorption number NSORPT in data block TRACR are in conflict. For example, setting TRTYPE = 'C' and NSORPT<7 shall cause an error message to be printed and the simulation to be aborted.
10. If the character variable LPTYPE \neq 'stfs' and LPTYPE \neq 'hoog', indicating that the numerical inversion method of the Laplace space solution is to be neither the Stehfest algorithm nor the De Hoog method.
11. If a tracer is declared a parent or a daughter in a radioactive chain (PCTYPE = 'P' or PCTYPE = 'D') and its molecular weight WTMOL=0.
12. If the number of active dimensions NACTDI (determined internally by EOS9nT from the input file) (a) is different from 1, 2 or 3, or (b) exceeds the maximum value NDIM declared in TRCOMN.f.

ATTACHMENT C INSTALLATION TEST LOG

The tester shall document the results of the installation test case execution in the Installation Test Case Log below. In that table, the tester shall record results that include pass/fail annotation with initials and date.

Table C.1 Log of Installation Test Result

InfTest	Pass/Fail	Initials	Date

ATTACHMENT D VALIDATION TEST CASES

Validation test cases were described in Section 5.2 of the Design Document for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-DD-1.11MEOS9NTV2.0-01), and the results of the execution of the Test Plan followed the approved plan contained in the Design Document are available in Section 4.1 of the Software Validation Report for TOUGH2 V1.11MEOS9NT V2.0 (Document ID: 10065-SVR-1.11MEOS9NTV2.0-01).

The following general process will be followed:

- (a) Transfer from the distribution media 10065-MED-1.11mEOS9nTV2.0-00 the archived file for the appropriate platform (Unix) and install the software as will be described in the Installation Test Plan (ITP) 10065-ITP-1.11mEOS9nTV2.0-00. The six directories containing the VTP test cases are in directory TestProblems.

- (1) Test#1_F
- (2) Test#2_F
- (3) Test#3_F
- (4) Test#4_F
- (5) Test#5_F
- (6) Test#6_F

- (b) The input files may have one or more of the following suffixes:

- (1) “_T”: denoting conventional time stepping
- (2) “_S”: Laplace transform formulation, Stehfest algorithm
- (3) “_H”: Laplace transform formulation, DeHoog formulation

- (c) For each test, name the output file by attaching the “.outX” suffix to the input file name. Run the code as instructed shown below in the Table 1. Move the output into the corresponding folder, and compare the results to

- (1) The reference output file (designated by the “.out” suffix) – obtained by running the same test problem using EOS9nT v2.0 (output obtained by the developer, and provided on the distribution media)
- (2) Where applicable, the regression output file (designated by the “.outR” suffix) – obtained by running the same test problem using the qualified TOUGH2 V1.11mEOSE9nT V1.0 software (software identified in each case, and input/output provided on the distribution media)
- (3) Unless otherwise specified, the acceptance criterion is a difference of $\leq 5\%$ between (a) the predicted tracer mass fractions from the simulation results and from the reference results when the relative mass fraction (ratio of final to initial mass fraction) exceeds $1.0E-5$, or (b) the predicted distance from the origin of the concentration front (designated as the point when the relative mass fraction is $1.0E-5$) obtained from the simulation results and from the reference results.

Table 1 Example Run for Execution Instruction

Step	Installation Activity	Expected results
1. Changing directory	“cd” to the installation test directory cd ../TestProblems/Test#N_F	Directory changed.
2. Execution	Run T2E9nTx from the command line, designating “Test_N_X.out” as the output name (see attachment for detailed description). ../EOS9nTv2.0_Code/T2E9nTx < Test_N_X > Test_N_X.outX,	No execution error occurs.
3. Comparison	Compare “Test_N_X.outX” to the reference output files ““Test_N_X.out” and “Test_N_X.outR.out”.	The file comparison meets the acceptance criteria described below in this section
Notes: 1. “N” represents the test case number, “1b” for test 1, “2” for test case 2, “3b” for test case 3, “4”, “5”, or “6” for test cases 4, 5 or 6, respectively. 2. “X” represents “H” for deHoog, “S” for Stehfest, or “T” for timestepping		

If the comparison of the results of the validation test output file and those in the reference output file provided in the installation media shows that

The quantitative acceptance criteria for all cases are for the EOS9NT is listed as follows:

- (a) Using an initial reference mass fraction of 1, when the mass fraction in the new output file, for example "Test_1b_H.out" and the reference output file, for example "Test_1b_H.outR.out" are larger than 1.0e-6, the mass fractions in new output file and the reference file differ less than 5%, or
- (b) The mass balances of the tracers differ by less than 5%

D.1. Test Case 1 (TC-01)

Transport of a Non-Sorbing, Non-Radioactive Solute

This problem shall examine the transport of a single non-sorbing stable isotope ($\lambda = 0$) in a fully saturated, semi-infinite horizontal medium (*Bear, 1979*). The groundwater pore velocity is to be $V = 0.1$ m/day, the dispersion coefficient is to be $D = 0.1$ m²/day, and the porosity ϕ is to be 0.3. A uniform grid size of $\Delta x = 1$ m is to be used. Concentration profiles are to be obtained at $t_1 = 50$ days and $t_2 = 400$ days.

Two sets of three runs each are to be conducted for the T, S, and H solutions. For the t_2 profile, an additional test is to be performed in this study to evaluate the ability of the De Hoog algorithm to obtain accurate solutions both (a) at the two specified times t_1 and t_2 and (b) at any time t in the interval $[0; t]$ from the solution at t . Thus, the concentration profile at $t = 50$ days is to be obtained from both the t_1 and the t_2 solutions.

The four (at t_1) and 3 (at t_2) solutions are practically identical, differing in the 3rd decimal place. This test confirms the validity of the 3 solutions, and the ability of the De Hoog method to provide accurate results within the solution period. Figure 1 shows a comparison between the numerical predictions (symbols) and the analytical solutions [Bear, 1979]. We observe an excellent agreement (< 5% difference in tracer relative concentrations) between the two sets of solutions. For clarity, the four coinciding solutions are represented by a single symbol.

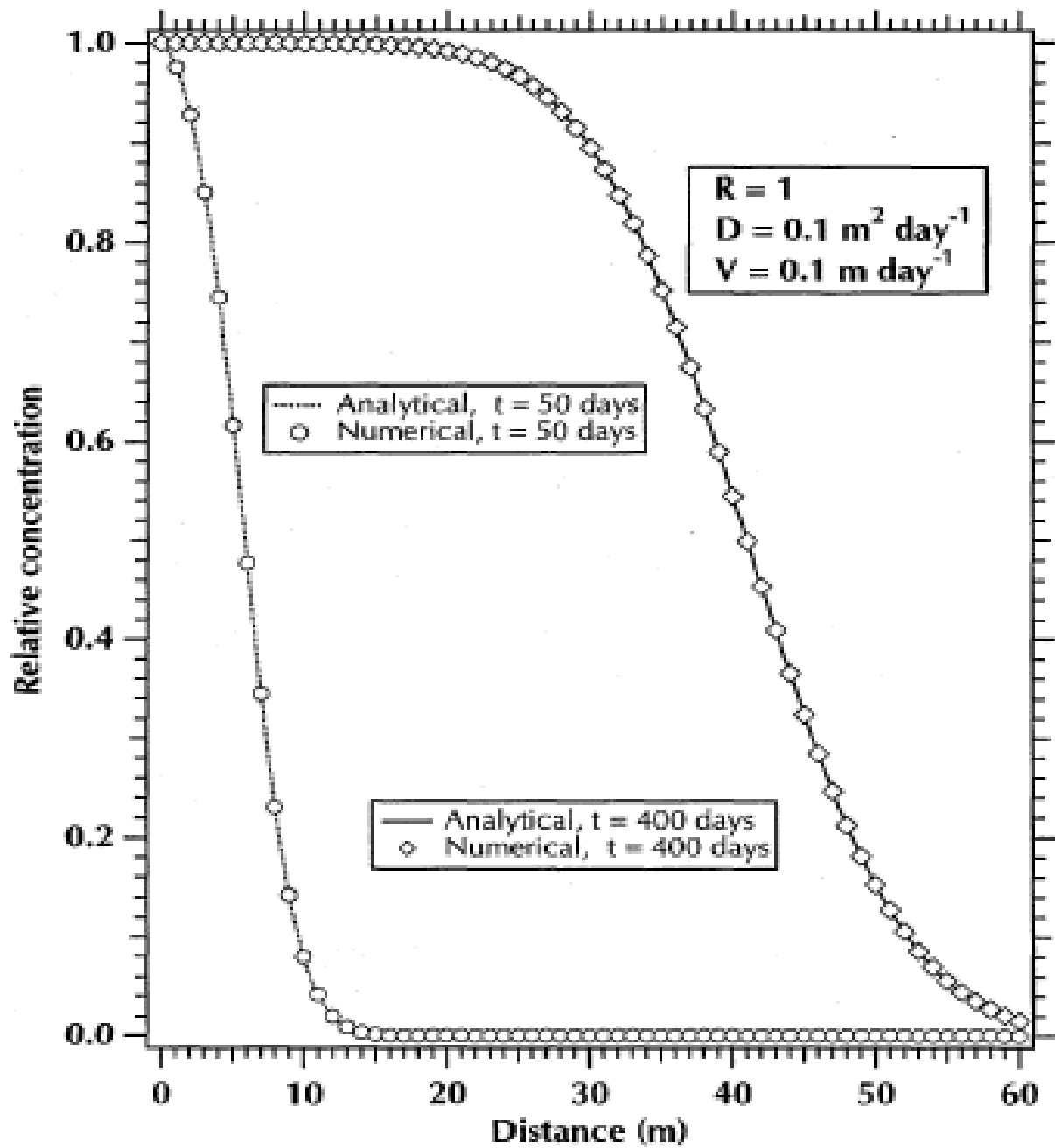


Figure 1. Analytical and numerical solutions at two different times of a non-sorbing, non-radioactive tracer in a semi-infinite column.

D.2. Test Case 2 (TC-02)

Transport of Radioactive Parents and Daughters in Porous Media

Test Problem 2 is planned to describe the migration behavior of the decay chain $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$ in a saturated porous medium (Harada et al., 1980). The most important species is ^{226}Ra because it is very mobile in geologic media and has high biohazard potential.

The half-lives of ^{234}U , ^{230}Th , and ^{226}Ra are 2.44×10^5 , 7.7×10^4 and 1.60×10^3 years, respectively. All three species are strong sorbers, with retardation coefficients $K_d = 10^4$ for ^{234}U , 4×10^4 for ^{230}Th and 5×10^2 for ^{226}Ra . In this problem, the other transport parameters are to be the groundwater velocity $V = 100$ m/yr, and the dispersion coefficient $D = 2.74$ m²/day.

At $t = 5 \times 10^5$ years, the agreement in Figure 2 between the analytical solution and the EOS9nT solution with the DeHoog formulation (denoted as EOS9nT-H in Figure 2) for all three species is excellent ($< 5\%$ difference in tracer relative concentrations). The same is not observed when the Stehfest formulation is used in EOS9nT (denoted as EOS9nT-S). Figure 3 shows that the agreement between the analytical solution and the EOS9nT-S predictions of ^{234}U distribution is excellent up to a distance of 1000 m, but exhibits an oscillatory behavior past that point. The comparison of the ^{230}Th and ^{226}Ra curves to the analytical solutions shows very large deviations.

The main reason for the deterioration in the performance of EOS9nT-S is inaccuracies introduced to the solutions via two ways. The first is the very large observation time, which causes roundoff errors in the computations. The second is that the Stehfest algorithm ignores the imaginary part of the Laplace parameter s , which can cause serious problems. These errors are very significant because their effect is amplified as the Laplace space solutions are inverted, and are attested to by the very erroneous solutions for ^{230}Th and ^{226}Ra . This is the reason why the convergence criterion for the PCG tracer solutions in the Laplace space is 10^{-12} , but only 10^{-6} in regular time-stepping.

In our experience, the Stehfest algorithm is very powerful, simple and fast for the simulation of any solute or colloid problem when $t > 1000$ years, but its performance can deteriorate fast past that point. This deterioration is not problem specific, but is numeric in nature and due to the reasons discussed above. For $t < 1000$ years, the Stehfest formulation yields accurate predictions of parent transport, but it is inadvisable to track daughter transport because the small errors in the solution for the parent are sufficient to contaminate the solution for the daughters. On the other hand, the De Hoog formulation is free of these problems for parents or daughters, and yields accurate solutions for any time we have tried.

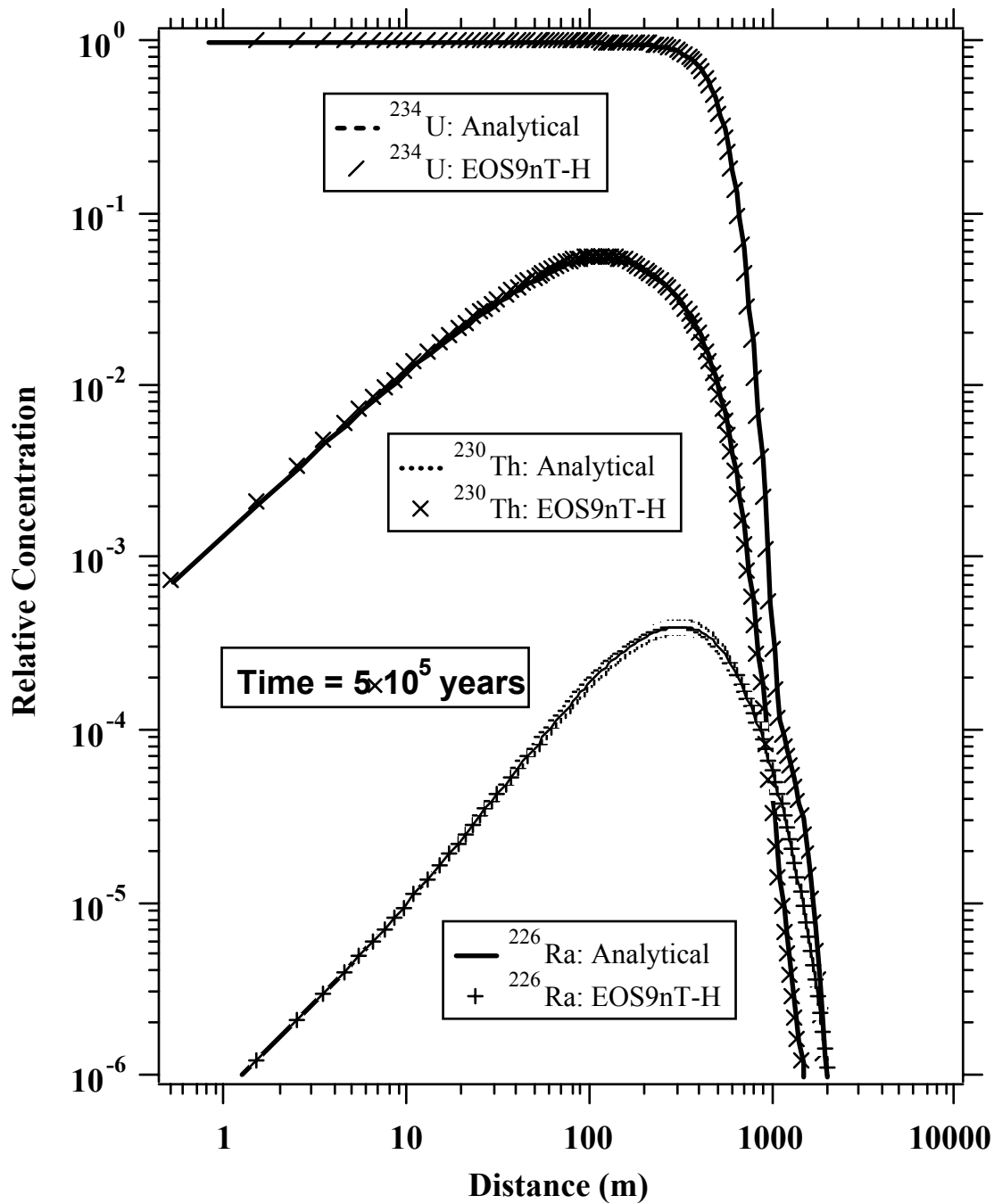


Figure 2. Comparison of analytical predictions of the concentration profiles of the species in the decay chain $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$ to the EOS9nT solution with the De Hoog method for Laplace formulation.

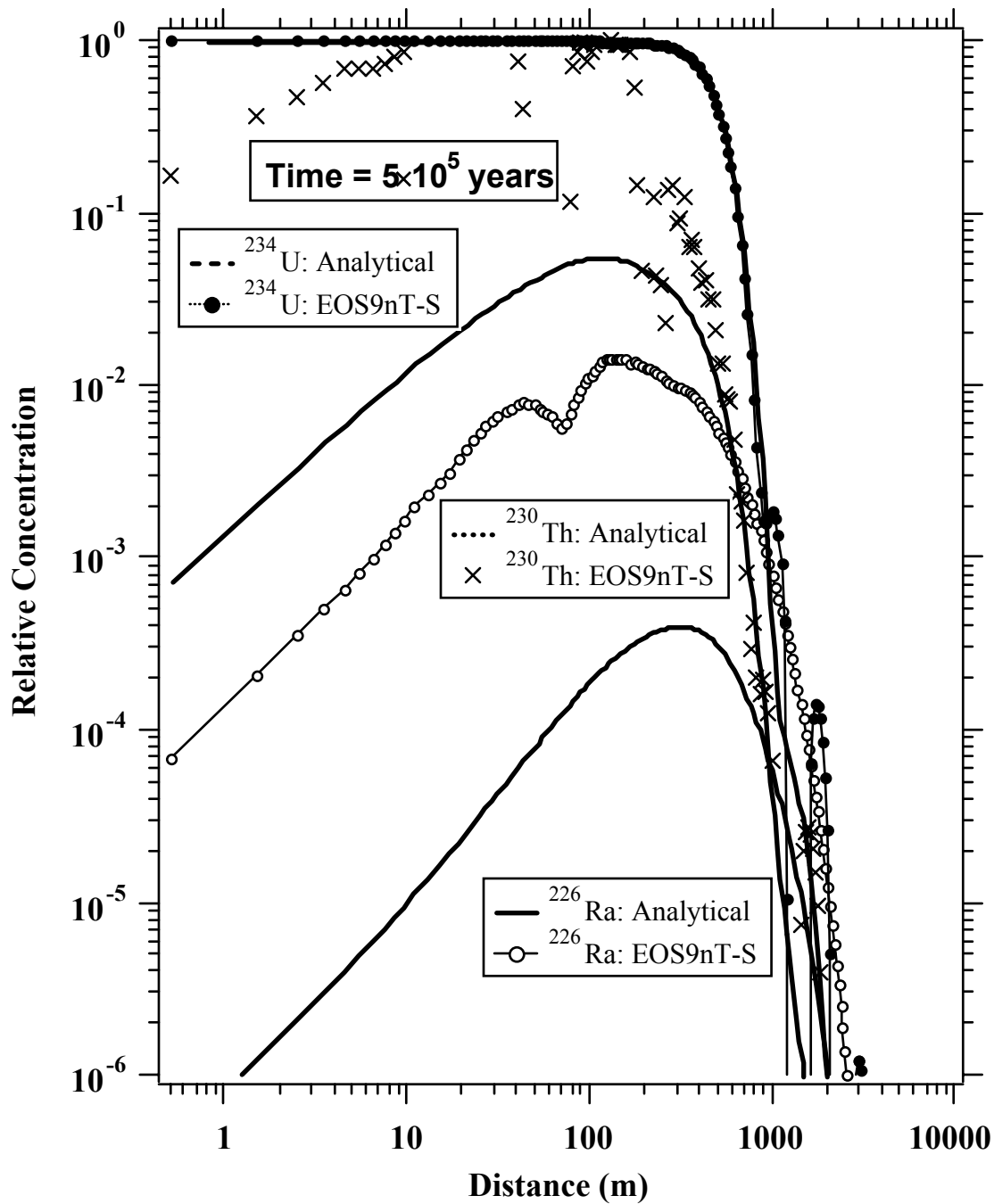


Figure 3. Comparison of analytical predictions of the concentration profiles of the species in the decay chain $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$ to the EOS9nT solution with the Stehfest algorithm for Laplace formulation.

D.3. Test Case (TC-03)

Transport of Radioactive Species in Fractured Media

The transport of radionuclides in fractured media in Test Problem 3 are planned to involve a single fracture and a matrix block of finite thickness. The analytical 2-D solution to this problem was developed by *Sudicky and Frind* [1982], and assumes only diffusion but no advection through the matrix.

The parameters used in Test Problem 3 are those of the large fracture-spacing case in the *Sudicky and Frind* [1982] paper. The fracture width $2b = 100 \mu\text{m}$, the matrix porosity $\phi = 0.01$, the matrix tortuosity $\tau = 0.1$, the fracture longitudinal dispersivity $\alpha_L = 0.1 \text{ m}$, and the diffusion coefficient $D = 1.6 \times 10^{-9} \text{ m}^2/\text{s}$. The species is to be a non-sorbing radionuclide ($R = 1$) with $T_{1/2} = 12.35 \text{ yrs}$. The water velocity is to be $V = 0.1 \text{ m/s}$, and the matrix block width is to be $2B = 0.5 \text{ m}$.

Three different 2-D grids in (x, z) are to be used for the EOS9nT simulations, with increasing finer discretization in the matrix block. The discretization of the coarse grid is to be set at 2×320 in (x, z) , with the fracture and the matrix each occupying a single gridblock at any z level. The discretization of the medium and the fine grids are to be 5×320 and 12×320 in (x, z) , respectively.

Figures 4 through 7 show the concentration distribution in the fractures at $t = 100, 1000, 10,000$ and $100,000$ days. All 3 EOS9nT solutions (i.e., T, S and H) for all discretizations are represented in the figures, as their results were extremely close ($< 5\%$ difference in tracer relative concentrations). The comparison to the analytical solution shows that the coarse grid yields inaccurate results, which tend to indicate an early breakthrough. The medium and fine grids, however, return very accurate solutions which are very close to each other.

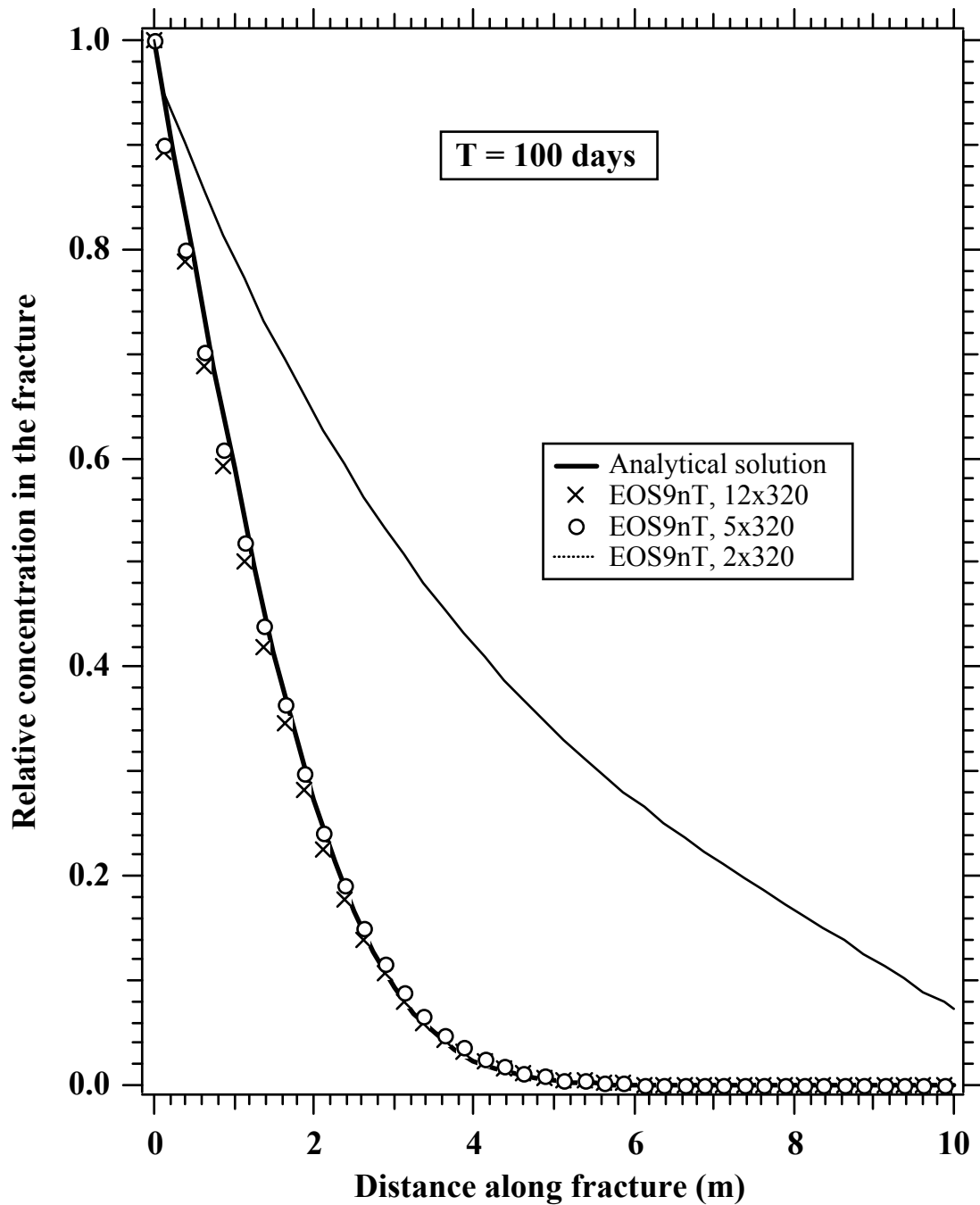


Figure 4. Analytical and numerical solutions of the concentration distribution in a fracture for three different grids at $t = 100$ days. The error caused by the coarse discretization accuracy is significant. The solutions for a medium and fine grid are indistinguishable.

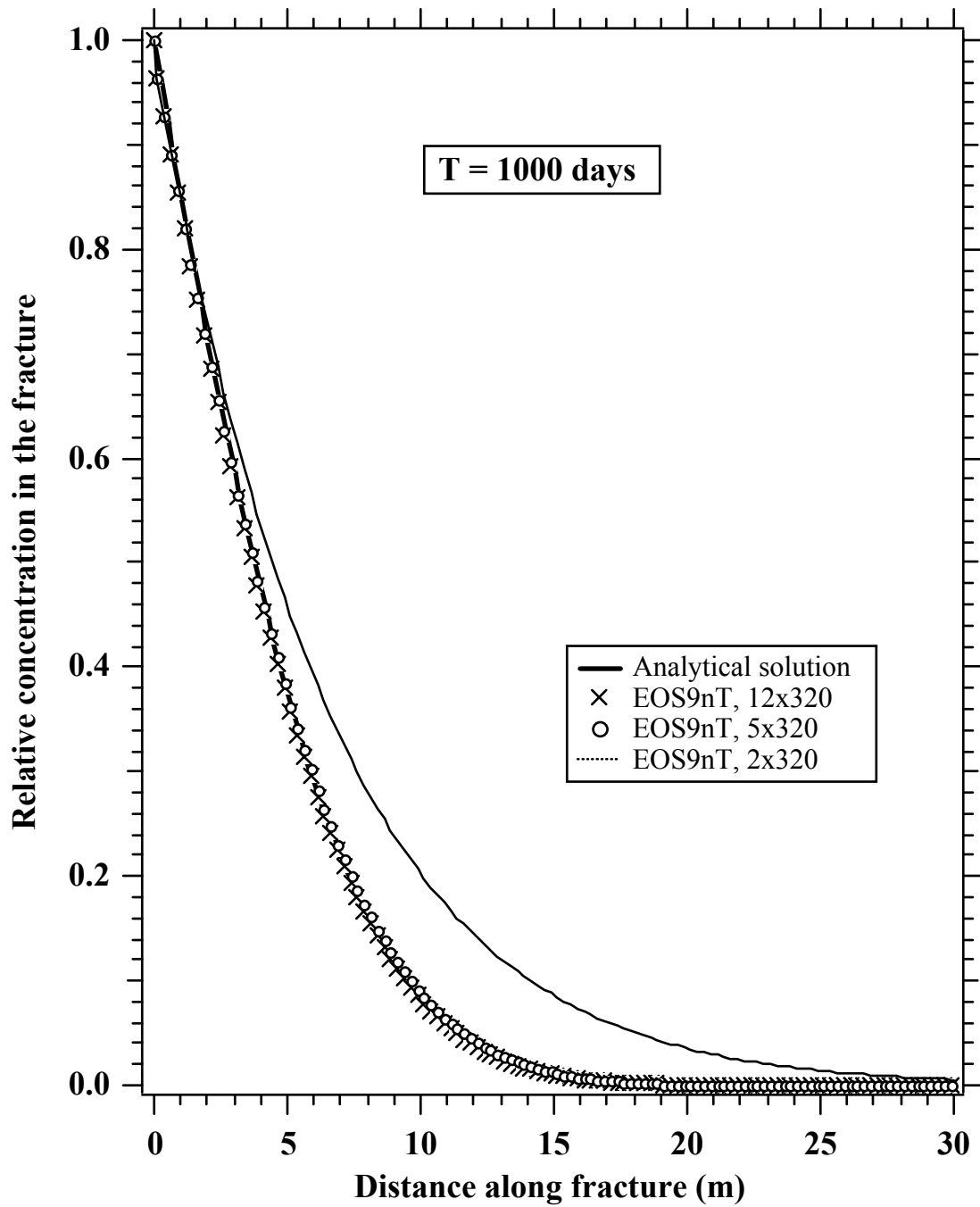


Figure 5. Fracture concentration distribution at $t = 1000$ days. The deviations between the numerical solution for the coarse grid, and the ones for the medium and the fine grids, are becoming smaller.

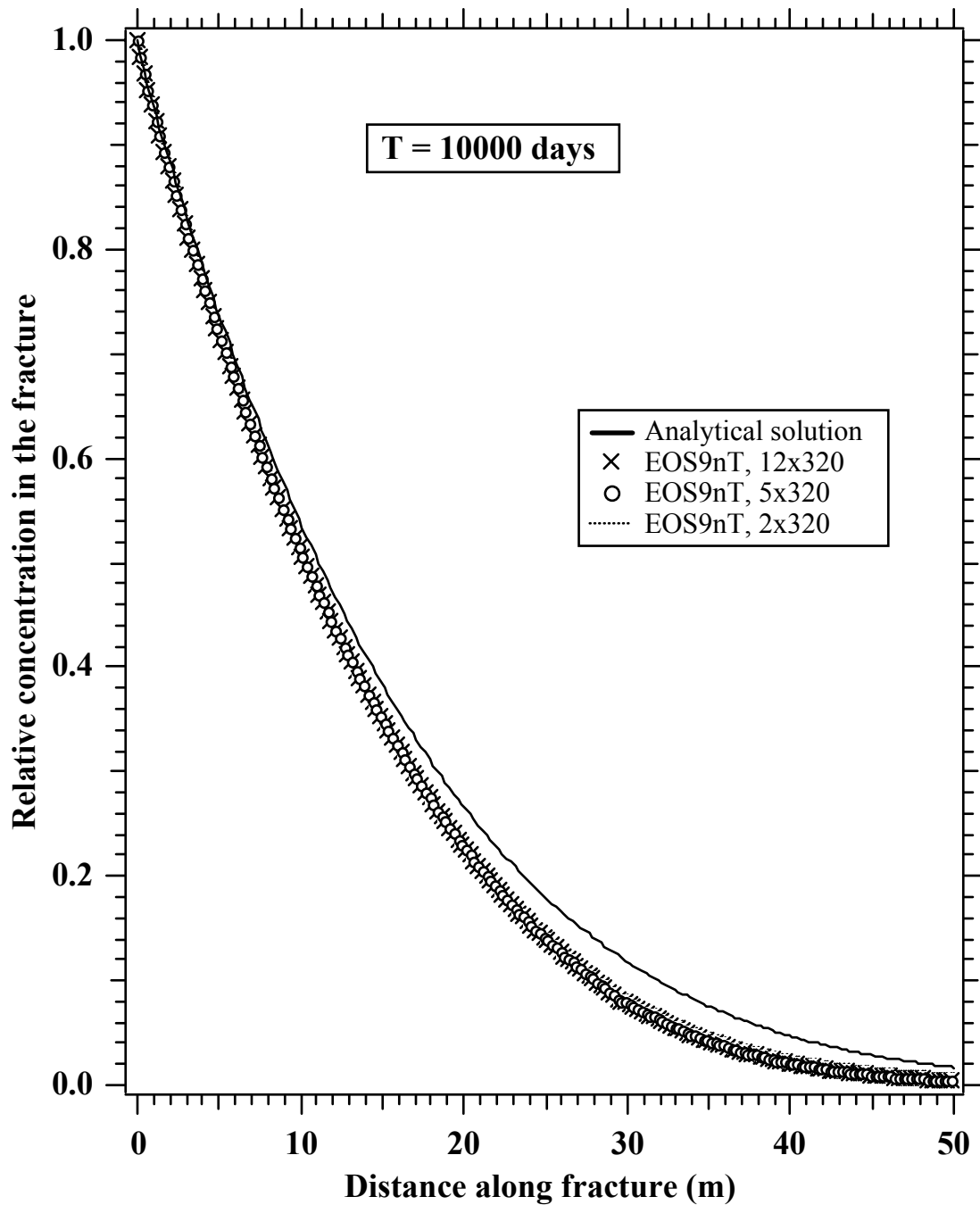


Figure 6. At $t = 10,000$ days, the EOS9nT solutions with medium and fine grids coincide with the analytical. The deviation of the solution for the coarse grid is still measurable, although much smaller than at earlier times.

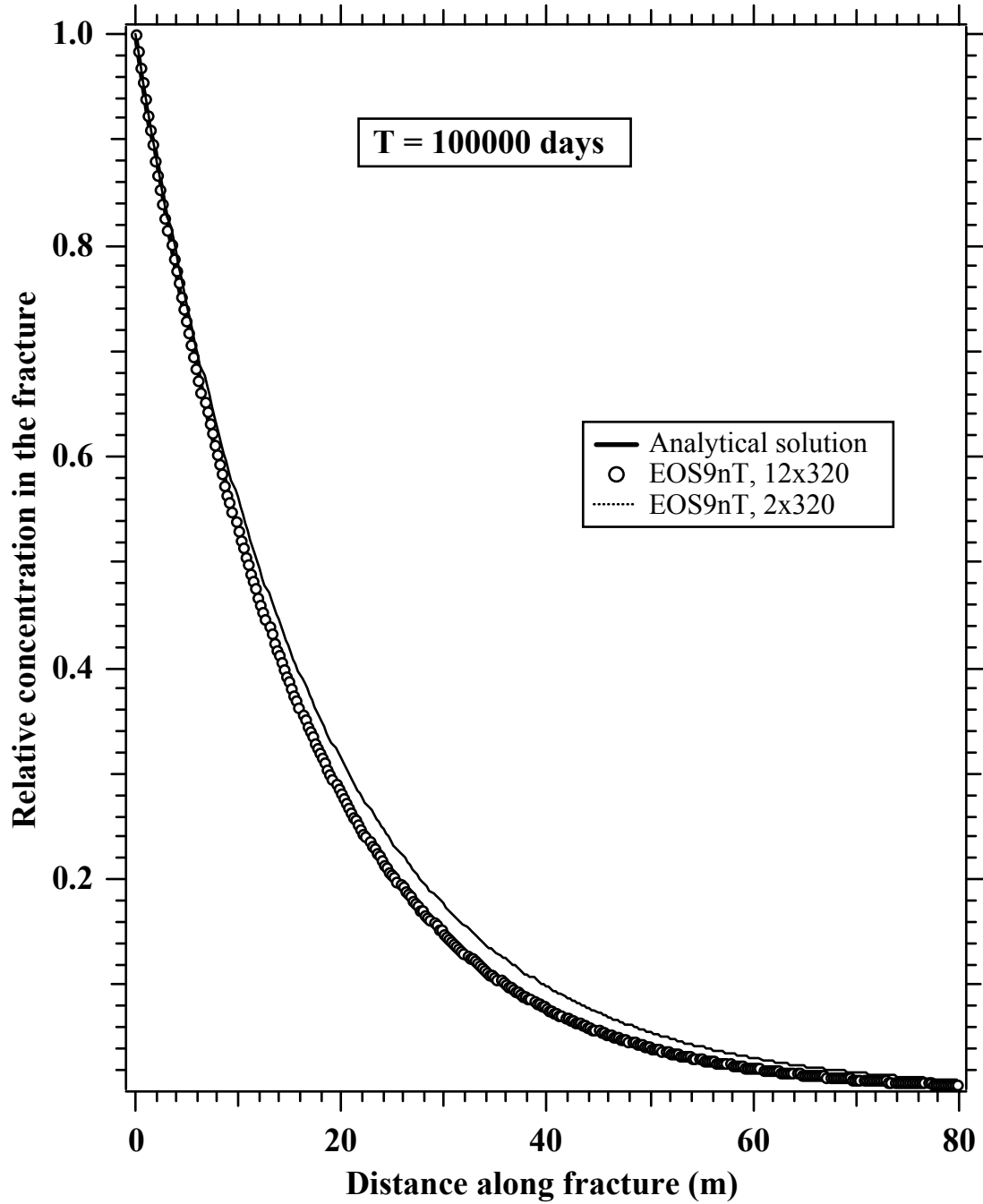


Figure 7. At $t = 100,000$ days, the coarse grid solution converges with all the other solutions.

D.4. Test Case 4 (TC-04)

Flow and Transport into an Unsaturated Column

Test Problem 9 is to be the horizontal infiltration problem originally solved by *Philip* [1955]. A semi-infinite horizontal tube filled with a homogeneous soil is to be partially saturated with water. The soil porosity is to be $\phi = 0.45$, and the initial moisture content is to be set as $\theta = 0.2$, corresponding to a liquid saturation of $S_w = \theta/\phi = 0.44$. The liquid saturation at the $x = 0$ boundary is to be held constant at $S_w = 1$ for $t > 0$. Due to a capillary pressure differential, water infiltrates into the horizontal system. Air is to be considered a passive phase, and its effects are neglected.

The problem is to be augmented by adding two tracers to the water at the $x = 0$ boundary. The mass fractions of the first and second tracers are to be $X_1 = 10^{-3}$ and $X_2 = 10^{-4}$, respectively. Note that, because of linearity, any value can be used for X , and $X = 1$ is very convenient. The first tracer is to be non-decaying, and have an $R = 2$. The second tracer is to be non-sorbing ($R = 1$) and have a $T_{1/2} = 1$ day.

Because of the unsaturated conditions and the non-linearity of the problem, the Laplace transform formulations cannot be used, and only the time-stepping solution is to be employed. Using the EOS9nT module and the EOS7R module [*Oldenburg and Pruess, 1995*], solutions are to be obtained at $t = 0.01$ day, $t = 0.06$ days, and $t = 0.11$ days. A uniform grid size of $\Delta x = 0.002$ m is to be used.

In Figure 8 we compare the numerical (EOS9nT and EOS7R) and analytical solutions of saturation *Philip* [1955] at the three observation times. The two sets of solutions are in excellent agreement ($< 5\%$ difference in tracer relative concentrations). Figures 9 and 10 show the EOS9nT and EOS7R solutions of the concentration distributions of the two tracers at the same times. The EOS9nT and EOS7R solutions were identical in all cases.

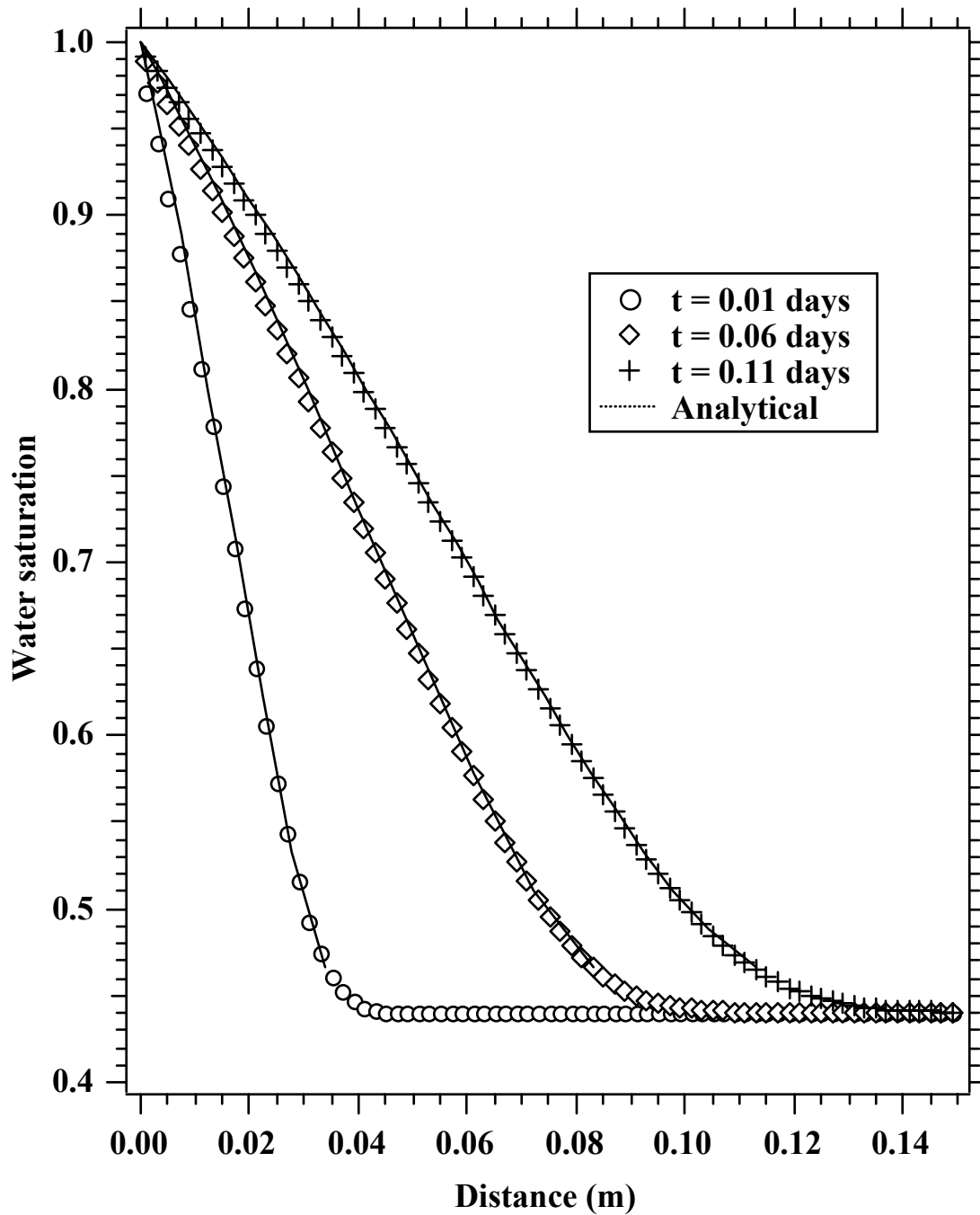


Figure 8. Analytical and numerical solutions of the water saturation distribution in Test Problem 9.

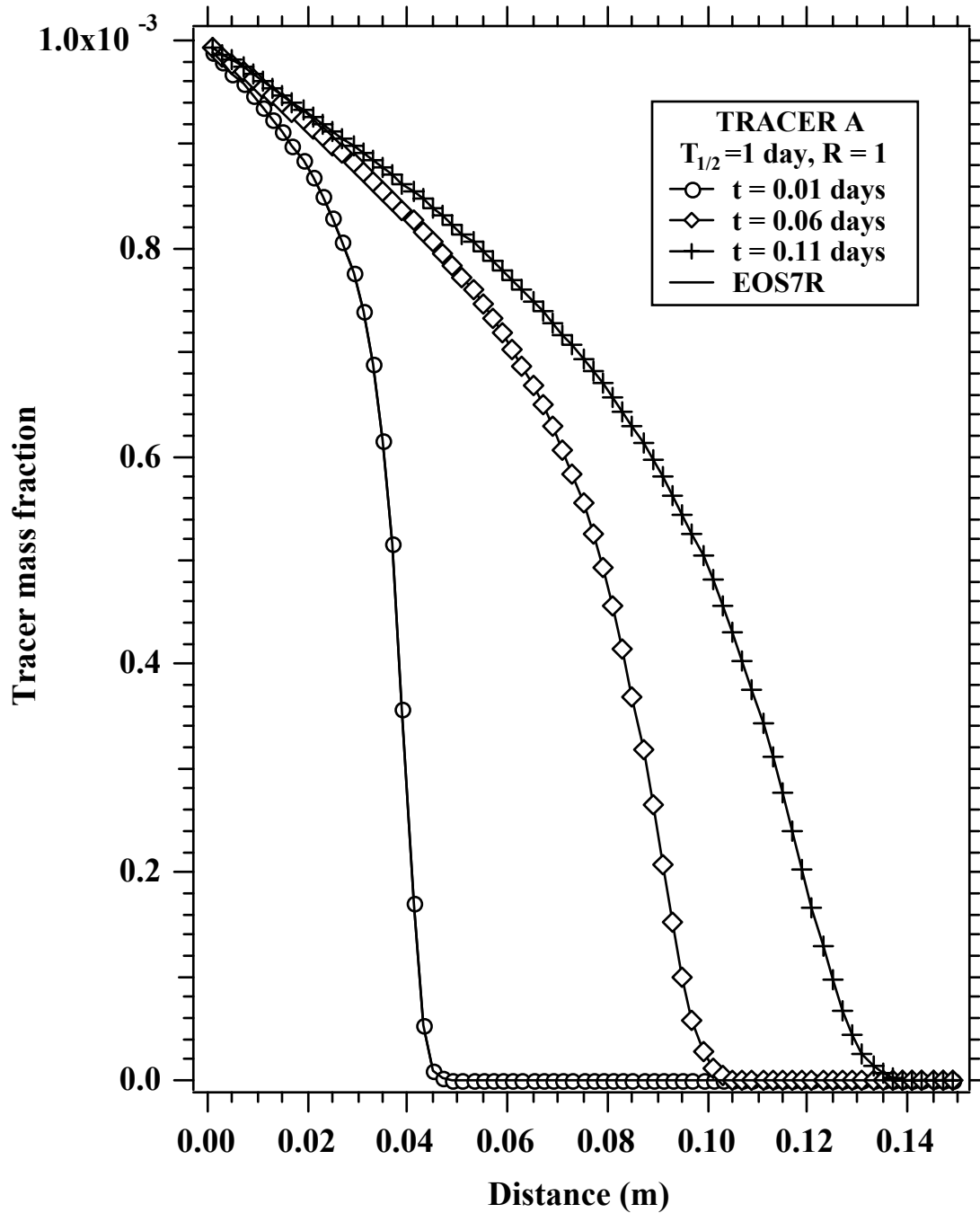


Figure 9. Numerically predicted concentration of a sorbing non-decaying tracer using the EOS9nT and the EOS7R modules.

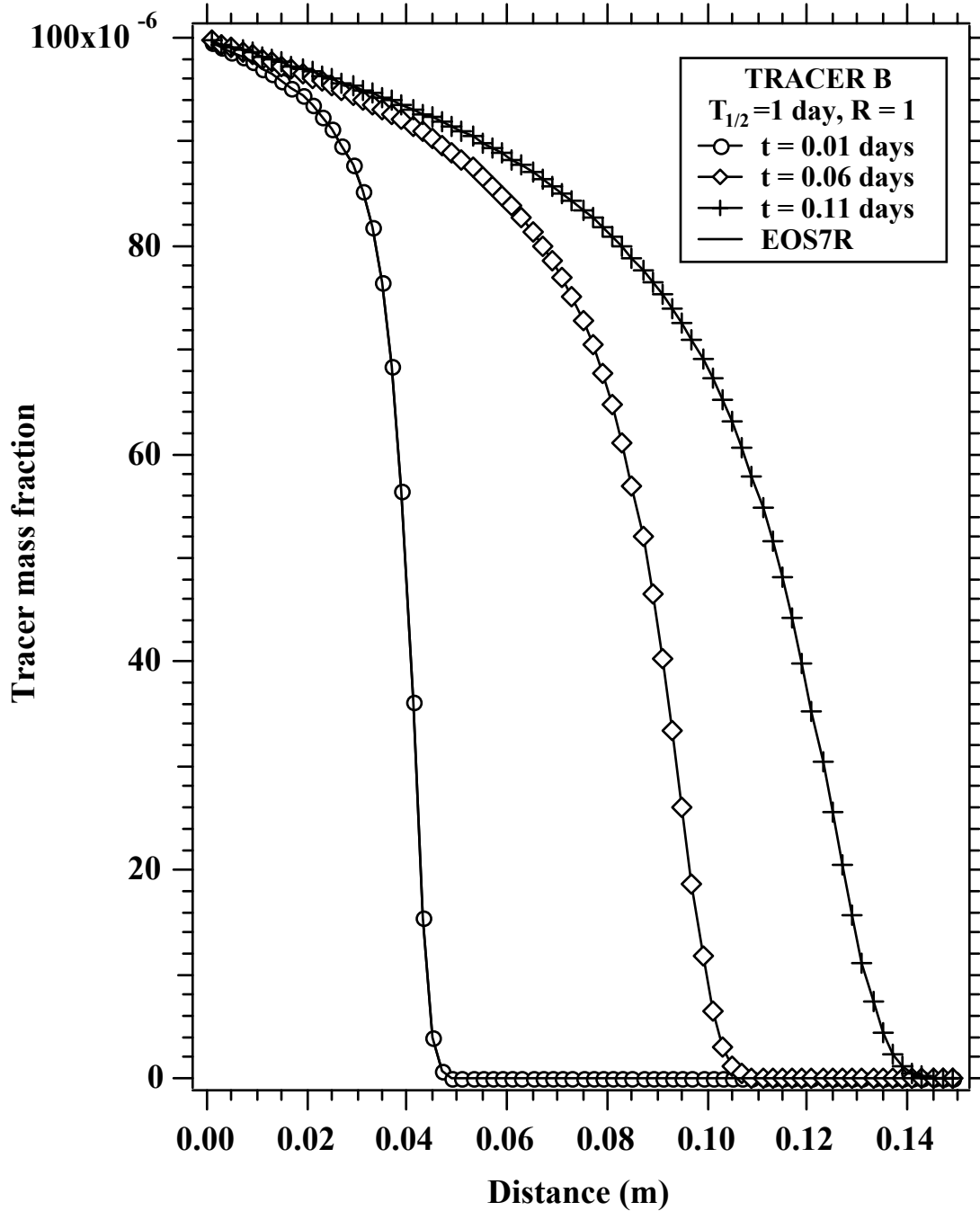


Figure 10. Numerically predicted concentration of a non-sorbing radioactive tracer using the EOS9nT and the EOS7R modules.

D.5. Test Case 5 (TC-05)

Simultaneous water flow and tracer transport through an unsaturated medium (8-character element names)

This problem involved transport of a nonsorbing, nondecaying tracer after instantaneous release through a porous medium along a 1-d column at Yucca Mountain.

The two codes, T2R3D V1.4 and TOUGH2 V1.11MEOS9NT V2.0 have been shown to produce identical results in simulations of transport involving (a) conventional time stepping and (b) nonsorbing tracers or tracers whose sorption follows an equilibrium linear sorption model. A comparison of the performance of the two codes is shown in Figure 11, which depicts predictions of transport of a conservative (nondecaying, nonsorbing) tracer along a vertical column of Yucca Mountain. A family of analytical solutions to this problem were developed by Bear (1979 [105038]). The properties and parameters for this problem are listed in Table 1

Table D.5.1 Parameters in Test #5

Parameter	Value
V (m/day)	0.1
D (m^2 /day) - Equation 20	0.1
K_d (m^3 /kg)	0
Water saturation S_w	1
τ	1

Figure 12 shows a comparison between the analytical solution and the numerical model predictions, and includes solutions from three different time treatments (designated by T, H, S to indicate regular time stepping, De Hoog Laplace space solution and Stehfest Laplace space solution, respectively, see Attachment I). Note that the results for regular time stepping (i.e., the T-solutions) reflect both the EOS9nT and T2R3D estimates, which are not shown separately because they are practically indistinguishable from each other, and from the Laplace space formulation solutions.

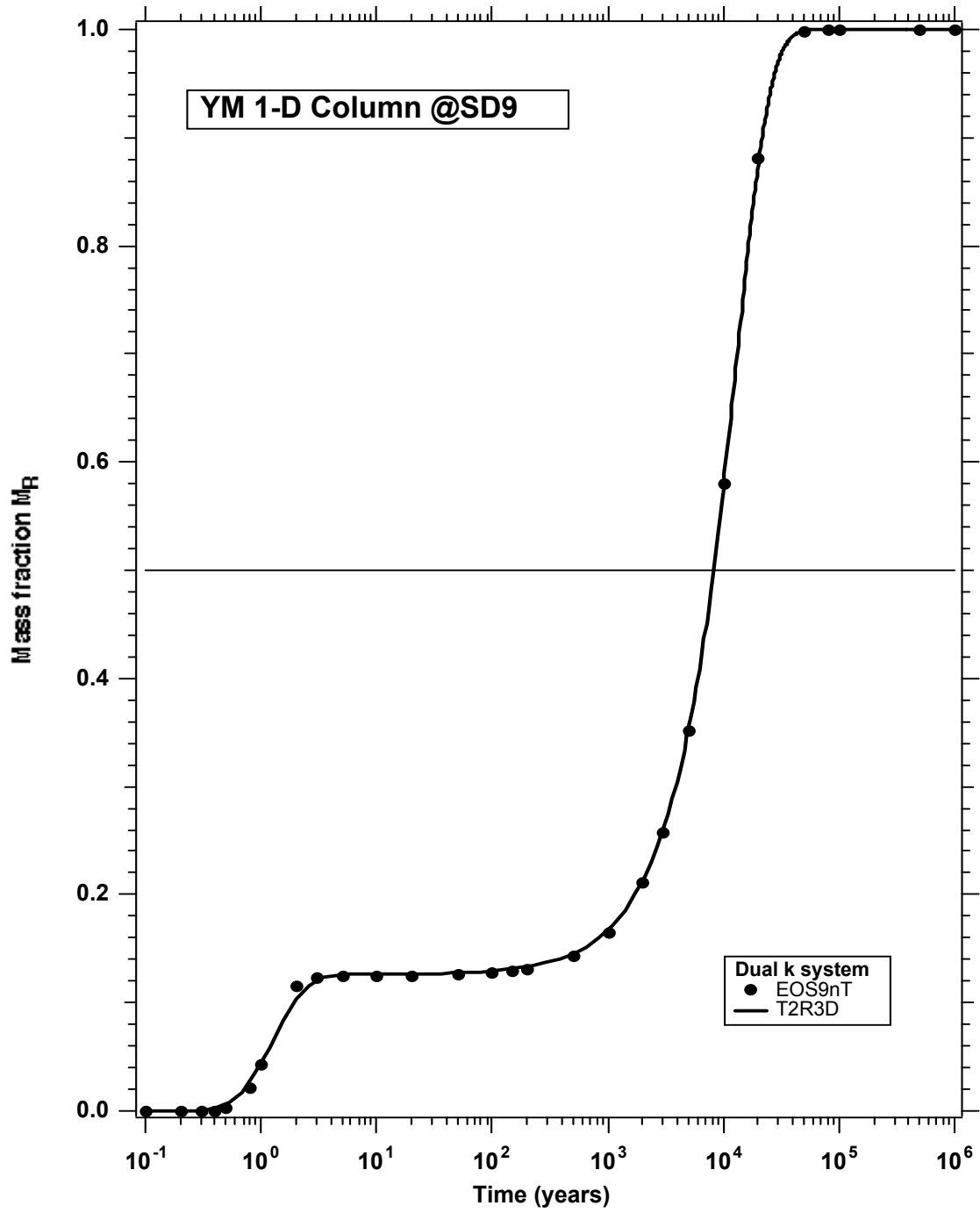
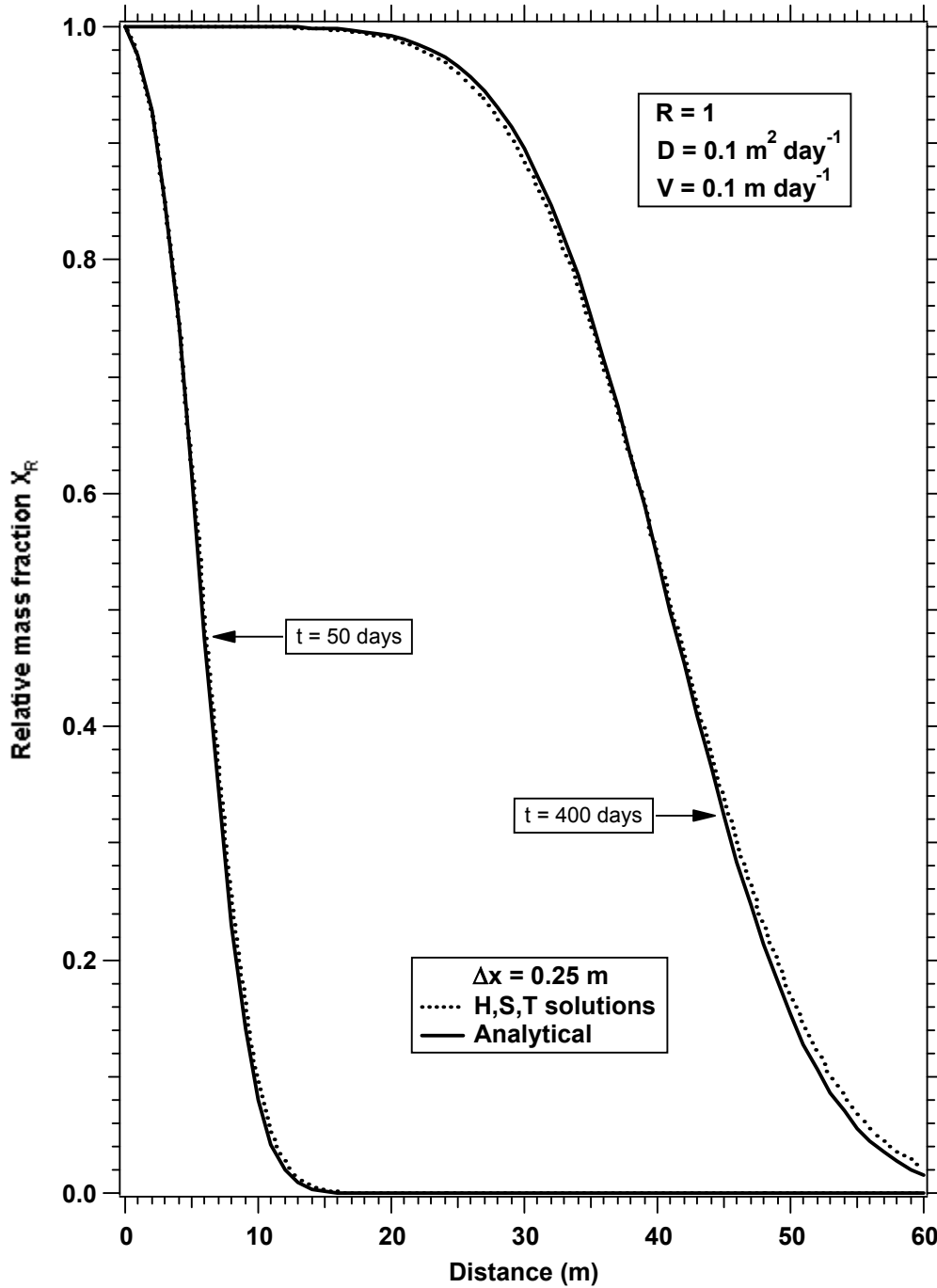


Figure 11. Comparison between the Numerical Predictions of Breakthrough from TOUGH2 V1.11 MEOS9NT V2.0 and from T2R3D V1.4.



NOTE: Note that the results from three different time treatments (designated by T, H, S to indicate regular time stepping, De Hoog Laplace space solution, and Stehfest Laplace space solution, respectively) are indistinguishable.

Figure 12. Comparison between the Analytical Solution and the Numerical Predictions in Test #5

D.6. Test Case 6 (TC-06)

Colloid Transport in Porous Media

Test Problem 6 is planned to study the transport of three non-sorbing, non-radioactive colloids in a saturated semi-infinite horizontal column. In most colloid studies it is assumed that filtration has an effect on both the porosity and permeability of the porous medium. Under the conditions and assumptions of this work, it is not the case here. An analytical solution of the flow and filtration of colloids without affecting the hydraulic properties of the medium is listed in *de Marsily* [1986], and considers only clogging without any mechanism for declogging.

The other parameters are to be groundwater velocity, $V = 2$ m/day, dispersion coefficient, $D = 1$ m²/day, and porosity, $\phi = 0.3$. The filter coefficients ε of the three colloids are to be set as 30 m⁻¹, 100 m⁻¹, and 3000 m⁻¹, respectively. A uniform grid size of $\Delta x = 0.01$ m is to be used. At $t = 7600$ s, the analytical and the numerical solutions of EOS9nT (T, S and H) in Figure 13 practically coincide.

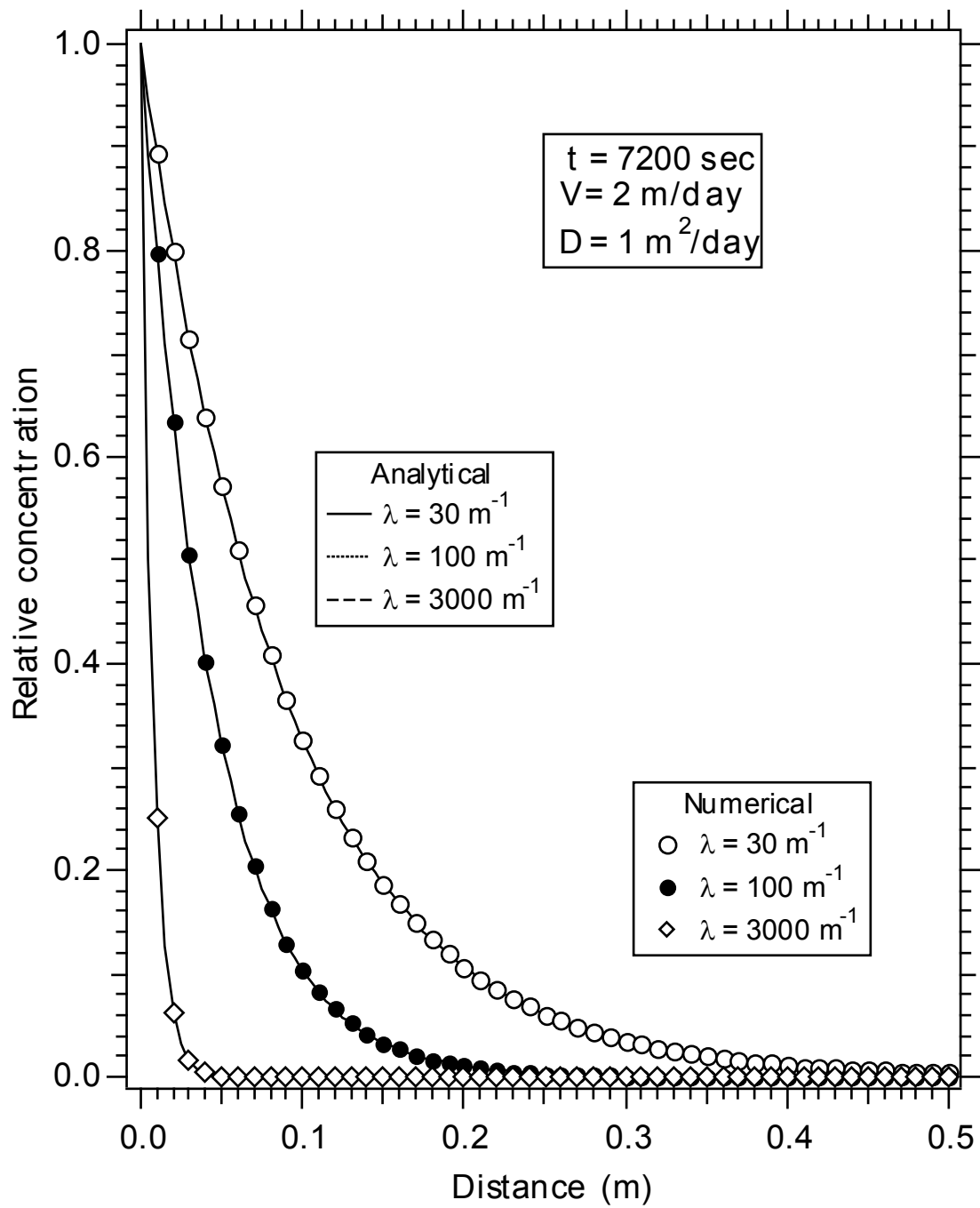


Figure 13. Analytical and numerical predictions of the concentrations of three non-sorbing, non-radioactive colloids.

ATTACHMENT E VALIDATION TEST LOG

Table E.1 TOUGH2 V1.11MEOS9NT V2.0 Validation Test Case Log

Tester Name:

Date:

Test Case ID	Pass/Fail (P/F)	Comments/Results
TC-01		
TC-02		
TC-03		
TC-04		
TC-05		
TC-06		