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MEMORANDUM FOR: Malcolm R. Knapp, Chief
Geotechnical Branch
Division of Waste Management, NMSS

THRU: Myron Fliegel, Section Leader
Hydrology Section
Geotechnical Branch
Division of Waste Management, NMSS

FROM: Richard Codell
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Geotechnical Branch
Division of Waste Management, NMSS

Peter Ornstein
Hydrology Section
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Division of Waste Management, NMSS

SUBJECT: TOUGH CODE CHECKOUT

At your request, we have successfully completed the checkout of the TOUGH code in order to determine its ultimate usefulness to the Division for studying variably-saturated HLW repositories. We find that the code is worthwhile, and recommend that the technical assistance and research tasks associated with the code should go forward. The rationale for our conclusions is contained in the attached report.

This memorandum and its attachment satisfy OPS plan item 5313121.

Dick

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Enclosure:
TOUGH Code Checkout

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TOUGH CODE CHECKOUT

By Richard Codell and Peter Ornstien

INTRODUCTION

The candidacy of the NNWSI site as a possible location for a geologic repository for High Level Waste has compelled the Geotechnical Branch to consider models for predicting parameter behavior in variably-saturated media. The TOUGH code was identified by the staff as a highly-attractive model for predicting hydrological phenomena and heat transfer in variably-saturated media. Several efforts are under way at Sandia National Laboratories and Lawrence Berkeley Laboratories dealing with this code, and others are contemplated.

The purpose of the present review is to describe the staff's experiences with the TOUGH code, and to identify problems which have been encountered. Particular emphasis have been placed on identifying problems which might lead to a conclusion that the code would be inappropriate for studying nuclear waste repositories, and that efforts should be made to develop or identify another code.

The staff's experience with TOUGH are described in the following sections. Results obtained for standard benchmarking problems and somewhat realistic repository problems are presented, as well as comparisons to analytical solutions. While difficulties with the code have been identified, we have found no reason to suspect that TOUGH is fatally flawed, or could not be used for its intended purposes.

DESCRIPTION OF TOUGH

The TOUGH code (Transport Of Unsaturated Groundwater and Heat) is a computer program which solves the differential equations for heat, water vapor, liquid water and air in a variably-saturated porous medium. The program uses the integrated finite difference method of spatial discretization, which is suitable for time-dependent solutions in one, two or three dimensions, and any conceivable geometry. Time discretization allows explicit, time-centered, or fully implicit integrations with automatic adjustment of time steps. The program uses a proprietary subroutine package, MA28, for efficiently solving large sparse arrays of linear equations (Du80).

The TOUGH code allows very flexible specifications for permeability and porosity throughout the grid, but does not include the effects of hysterisis. Sources and sinks of heat or mass may be arbitrarily specified. The TOUGH code is not specifically designed for fractured porous media, but the way in which the grid structure is encoded allows the blocks representing fractures to be adjacent to blocks representing porous media. This technique has been demonstrated to work for the case of a geothermal reservoir (Pr83), but to the staff's knowledge, has not been applied to a repository simulation problem in fractured media.

Chronology of Staff's Experience with TOUGH

An approximate chronology of the staff's experience with the TOUGH code is given below:

Fall 1982: Formal contact with the TOUGH code author, Karsten Pruess at Lawrence Berkeley Laboratories (LBL) was made. Dr. Pruess communicated the

capabilities of the predecessor code MULKOM with regard to flow and heat transfer in the unsaturated zone.

Winter of 1983: a pre-exisiting contract with LBL was modified to allow Dr. Pruess to complete the code development of MULKOM (hereafter known as TOUGH), provide NRC with cursory documentation, transfer the code to the Brookhaven CDC-7600 and conduct a seminar on the use of the code.

August 1983: P. Ornstein, M. Weber, M. Gordon, J. Pohle, and T. McCartin of NRC, and P. Davis of Sandia National Laboratories, attended a seminar at LBL on the use of the TOUGH code. No formal documentation was available, but an informal package was prepared by Dr. Pruess for the seminar. The package contained a description of the modeling concepts, a rough user's guide, and several test problems.

September 1983: TOUGH was successfully installed and tested on the Brookhaven CDC-7600 system.

October 1983: P. Ornstein corresponded with the developers of the proprietary subroutine MA28 used in the TOUGH code. The nature of the proprietary restrictions was discussed.

Winter/Spring 1984: Experiments were performed with TOUGH. Several of the test problems were rerun. A waste canister problem and a repository-scale problem were formulated and run. An apparent bug was discovered which inhibited the resaturation of elements dried-out by the heat. Measures to correct this discrepancy were discussed with the code author and arrangements made to incorporate a fix. TOUGH was successfully installed on the NIH computer system. This version incorporated the aformentioned fix.

Experimentation with TOUGH was begun at Sandia National Laboratories under FIN A1266, "Risk Methodology Development for Waste Isolation in Alternative Geologic Media".

July 1984: P. Ornstein met with Karsten Pruess of LBL, and Gene Runkel and Dave Updegraff representing Sandia to discuss the formal initiation of documentation for the TOUGH code, fixing code errors, incorporating code improvements and resolving the problem of disseminating the proprietary code MA28. Plans to develop a self teaching curriculum during FY85 were discussed. This would be handled through a subcontract with Sandia under FIN A1158, "Technology Transfer." Verification and validation was planned under Sandia FIN A1166, "Maintenance of Computer Programs." Study of the usefulness of the code for modeling a repository in unsaturated tuff could also continue under Sandia FIN A1266.

Benchmark Problem

TOUGH was used to simulate the two benchmark problem for unsaturated flow contained in the NRC Benchmarking study (Ro82). The first benchmarking problem is that of a one dimensional isothermal wetting front propagating through the dry zone. This problem has a semi-analyical solution (Ph55).

The results of the TOUGH and analytical models using the coefficients specified in the NRC Benchmarking study (Ro82) are presented in Fig.1 . The agreement between the models is nearly perfect. It is interesting to note that special consideration was needed to account for the purging of air from the modeled grid in the TOUGH simulation.

The second benchmark problem, 4.2 in (Ro82), is for a two-dimensional, vertical/horizontal flow, with the propagation of a wetting front. This problem has no known analytical solution, but has recently been solved numerically in connection with the NRC contract on benchmarking (Co84c).

P. Ornstein has made qualitative comparisons of the results of the TOUGH code with results using the codes FEMWATER and SATURN presented in the draft Benchmarking study (Co84c), and found good agreement. Neither of the benchmarking problems considered the effects of heat, however and therefore did not fully test the capability of the TOUGH code.

Other Problems Solved

Other problems solved with TOUGH or its predicessor codes include a geothermal benchmark problem, a fracture flow prcblem which had a semi-analytical solution, and several unverified problems involving realistic repository situations for unsaturated media, done in connection with the August 1983 training course. A predecessor code, SHAFT79, was used with good success for a detailed modeling study of a real geothermal well field in Italy (Pr83). The SHAFT79 code had been benchmarked with other geothermal codes in an international exercise.

Pruess and Bodvarsson were reported to have used MULKOM, another TOUGH predicessor code, to study heat and fluid flow in the proposed BWIP site (Li84). This simulation was two-dimnesional, and emphasised the two-phase, water/steam behavior in the near vicinity of the waste packages in the initially-saturated rock.

Pruess and Wang were reported to have applied TOUGH to a study of waste packages in the Topapah Spring member at NNWSI (Li84). This case was for an infinite cylindrical source in an infinite medium, similar to, but simpler than the NRC canister problem discussed below.

NRC Numerical Studies

As a test of the capabilities of the TOUGH code, P. Ornstein conducted a study of the hydrologic and thermal regime surrounding a HLW repository located in an

unsaturated tuff environment (Or84). Two cases were considered; a single cylindrical canister and a complete repository. The rate of heat decay was for 10-year old spent fuel. Properties of the tuff were taken from (Mo83). Surface rechange of water in both cases was a steady 1.0 cm/year.

Canister Study

(1) Numerical Study

A single cylindrical cansiter was simulated using the TOUGH code in order to predict the conditions in the near-field, irrespective of the influence of other canisters. The canister was considered to be a cylinder 4 meters in diameter and 2 meters high, with an initial heat generation rate of 3.4 kilowatts.

The problem was set up with the TOUGH code to simulate cylindrical coordinates. The grid consisted of 10 radial elements by 17 axial elements, with closer spacing near the canister. The performance was modeled for times up to 2767 days. The temperature inside the canister block as a function of item is shown in Fig. 2. The maximum temperature of the canister reached 99.4°C at 508 days. The phenomenon known as "heat piping" was observed to occur. Water vapor was driven from the tuff close to the block by increased vapor pressure, and condensed in surrounding blocks. Heat piping is a potentially important mechanism for heat transfer, because considerable thermal energy is expended in vaporization and released in condensation, and the gas phase (i.e., water vapor and air) can move rather easily in the tuff because of the high pressure gradient and low viscosity of the fluid. Temperature as a function of distance from the source block at t = 2767 days is shown in Fig. 3.

(2) Analytical Study

No analytical (i.e., closed form) solution of the complicated phenomena involved with the simultaneous heat and mass transfer in variably saturated porous media is known to exist. It is instructive, however, to consider a simplified case considering only conductive heat transfer. The importance of other phenomena such as heat piping can be demonstrated by comparing the two results.

An analytical approach for calculating heat transfer in a saturated geologic repository was investigated by Codell (Co84a, Co84b). It was determined that heat transfer in a typical saturated repository would be dominated by conductive heat transfer, and that convective heat transfer would account for only a minor quantity of heat. A semi-analytical method was developed to calculate the three-dimensional temperature field surrounding a repository with uniform heat conductivity (Co84b).

A semi-analytical model was developed for the canister study from the model of (CO84b). The model uses the Green's function approach for an instantaneous heat source, in an infinite uniform medium, generalized with the convolution integral (Ca59). The Green's function for a cylindrical heat source is available but involves a rather complicated series, which might converge with difficulty. A far simpler representation of the source is an oblong shape, 3.54 x 3.54 x 2 meters, which has the same volume as the cylinder. The temperature resulting from an instantaneous heat load of one joule per cubic meter per year would be:

$$T_i = \frac{1}{8\rho c_p}\left[\mathrm{erf}\left(\frac{\frac{W}{2}+y}{\xi}\right)+\mathrm{erf}\left(\frac{\frac{W}{2}-y}{\xi}\right)\right]\cdot\left[\mathrm{erf}\left(\frac{\frac{L}{2}+x}{\xi}\right)+\mathrm{erf}\left(\frac{\frac{L}{2}-x}{\xi}\right)\right]\cdot\left[\mathrm{erf}\left(\frac{\frac{H}{2}+z}{\xi}\right)+\mathrm{erf}\left(\frac{\frac{H}{2}-z}{\xi}\right)\right] \qquad (1)$$

where,

$\xi = \sqrt{4kt}$, k = thermal conductivity, t= time,

L, W, H = length, width and height of canister,

ρ = bulk density of medium, c_p = bulk heat capacity of medium,

and x, y and z are the spatial ordinates.

For a time varying heat load, H(t) Eq. 1 can be generalized to:

$$T = \int_0^t H(t-\tau)\, T_1(\tau)\, d\tau \qquad (2)$$

A BASIC language program "TOUGHAN2" performs the numerical integration of the above equations. Since the canister geometrics was not identical in the two approaches, the temperature for the TOUGH approach was calculated at r = 1.0 meter, while the TOUGHAN2 temperature was calculated at x = 0.89 meters. These distances were chosen so that they were half way between the canister centerline and the edge of the canister.

Canister temperature calculated with the TOUGH code were, as expected, lower than the analytical results, demonstrating the heat loss caused by the phenomena of evaporation and heat piping. The temperature peaks for each model occured at approximately the same time, however, and the shape of the curves were very similar. Temperatures along the line x = 0, z = 0 and time = 2767 days for both the analytical and TOUGH approaches are shown in Fig. 3, and are nearly identical, especially a few meters away from the canister. It is likely that heat piping is important within a few meters of the canister, but heat transfer is dominated by conduction at larger distances. The relatively small quantity of water evaporated did not account for a significant temperature reduction except very close to the canister.

Repository Study

(1) Numerical Study

A repository scale problem was also simulated to investigate phenomena on a larger spatial and time scale. The repository was considered to be a

horizontal disk, 6.5 meters in thickness and 200 meters in diameter. Heat was generated at an initial rate of 100 KW/acre of plan surface area.

A period of 9867 days was simulated, at which point an aberration in the code was discovered, which would not allow previously-desaturated grid blocks to resaturate. A remedy for this problem has been implemented in the code.

Temperature near the center of the repository is shown in Fig. 4. The phenomenon of heat piping is observed with water evaporating near the heat source and condensing in cooler blocks further away. Liquid water moves toward the dried-out areas because of their lower matric potential. A sharp rise in temperature occurs at about 5800 days due to total desaturation of the rock near the repository center, and the loss of the evaporative heat sink. Saturation of blocks further away from the source increased because the water evaporated close to the source had condensed there. Temperatures close to the vertical axis are shown in Fig. 5.

(2) Analytical Study

An analytical model of heat transfer from the repository was developed along lines of the analytical model for the canister. The heat source was considered to be a thin disk with a uniform heat generation rate of q_1, joules/m^2 of repository plan area. For an instantaneous release of 1 joule, the Green's function for temperature along the repository centerline perpendicular to the disk is (Ca59):

$$T_i = \frac{q_i}{2(\pi k t)^{1/2}} \left(1 - e^{-a^2/4kt}\right) e^{-z^2/4kt} \qquad (3)$$

where a is the radius of the disk, and the other terms are as previously defined. The temperature is generalized for a continuous heat source using Eq. 2, and was incorporated into a BASIC language code "TOUGHAN."

Results of the TOUGHAN runs are shown in Fig. 4 and 5 along with the TOUGH results. Figure 4 shows the temperature in the center of the repository as a function of time. The analytical model as expected, predicts higher temperatures, because the heat loss due to evaporation and heat piping is not modeled. The two curves are in closer agreement after about 5800 days, once all of the water in the vicinity of the repository has evaporated. Figure 5 shows the vertical temperature profile through the center of the repository. The analytical solution at t = 9867 days predicts a temperature which is uniformly higher. The explanation for this discrepancy is that a relatively large quantity of heat would still be in latent form at this time, which is not taken into account by the analytical model. It is likely that agreement for longer times would be better, since the water vapor would eventually condense as the heat production declined.

The comparisons with the analytical models for these two cases indicates that the TOUGH code appears to behave predictably. The differences between the analytical and numerical models is explainable by the phenomena taken into account in TOUGH.

An interesting observation which can be drawn for these numerical experiments is that long term heat transfer appears to be dominated by conduction, even though the heat-piping phenomenon is known to be highly effective.

Potential problems

The only serious computational difficulty found by the staff was the anomoly which prohibited resaturation of dried-out grid blocks in the repository example. The fix for this problem is not difficult, and will be incorporated

into future revisions of the code. As mentioned previously, this fix has already been incorporated into the NIH computer version.

The greatest limitations on the use of the code are likely to be considerations of computational resources. The TOUGH code when applied to complicated problems is likely to tax the reasonable limitations of present-day computational ability, both in terms of core storage and run time. These problems are legend among unsaturated-flow codes, however, and are not peculiar to TOUGH (Lappala, 1981). The solutions for flow in unsaturated media are by nature very difficult because of the strong dependence of permeability and matric potential on moisture content. The nonlinear partial differential equations generally require iterative solutions. The TOUGH code generally employs an iterative solution for each time step. Each iteration requires a gaussian elimination of a large sparse matrix. Although efficient schemes are used wherever possible, run times for TOUGH are characteristically very long.

Examples of several problems solved by TOUGH or predecessors of TOUGH illustrate the extent of the problem. Pruess et. al. (1983) used SHAFT79 for a geothermal well field simulation. The three-dimensional grid consisted of 234 elements, covering an area of about 5 x 7 kilometers. The model was run for 243 time steps for a simulated total time of 15.5 year, and took 2267 seconds of CPU time on a CDC-7600.

The repository-scale model study performed by Ornstein consisted of 198 nodes (Or84). It was run for 27.1 years simulated time and took approximately 1600 seconds of CPU time of a CDC-7600. The estimated cost for a single such run on the Brookhaven computer would exceed $500.00. It should also be mentioned that this problem is a relatively simple representation which takes advantage of radial symetry in cylindrical coordinates, and does not represent the expected shape of a real repository.

D. Updegraff has been running TOUGH and has encountered similarly long run times (Up84). He ran a variably saturated problem in a tuff medium but without heat load. The problem had 180 elements, and took 563 CPU seconds to complete 192 iterations (1 step per iteration) on a CDC-CYBER 172, which is approximately as fast as a CDC-7600. He ran a similar problem with no heat load on the Los Alamos CRAY-1 (one of the fastest computers in the world). This problem had 698 elements and took about 59 CPU seconds per iteration.

The above examples illustrate that it would be difficult or impractical to use TOUGH to simulate a tuff repository for long periods of time, e.g., hundreds to thousands of years, although periods of up to about 100 years might be possible. For longer times, the spatial and temporal rates-of-change of the primary variables would decrease, allowing progressively larger time steps.

The cost of running these problems must be weighed against the usefulness of the results. It is presently difficult to justify routinely running such costly jobs considering the relative scarcity of fundamental data on variably-saturated sites, when far simpler computations would probably be adequate. The present usefullness of the TOUGH code is in studying phenomena which may not be intuitive, and for which analytical solutions would not be expected to illustrate.

The availability of more powerful computers might bring longer simulations within reason. It is also possible that greater computational efficiency could be obtained from the computational algorthms in TOUGH. A 3-d finite element code for variably-saturated flow and heat transport, FLAMINCO (Ge83), is touted to have high computational efficiency using the "Slice Successive Overrelaxation" algorithm, although it is impossible to make a direct comparison to TOUGH.

Cooley (Co83) discusses several procedures employed to efficiently solve the equations for variably saturated flow. He claims that the finite element

formulation yields nonlinear matrix equations which are inherently more stable than those obtained from integrated finite differences, which is the method employed in TOUGH. Cooley also claims that his solution of the nonlinear matrix equations using Newton-Raphson iteration combined with the strongly-implicit method is highly efficient.

Updegraff (Up84) suggested that the efficiency of TOUGH would be improved if a regular grid setup were employed rather than the highly-flexible arrangement of element connections. The former allows matrices with small bandwidths, while the latter generally yields unbanded N x N sparse matrices, where N is the number of elements. Although a special solver for sparse matrices is used, the matrices occupy large areas of core memory, and might make the programming of other more efficient numerical solutions difficult or impossible.

Updegraff also suggested that much greater efficiency might be possible on the CRAY-1 computer if TOUGH were reorganized to "vectorize" the numerical algorithms, since the CRAY is well-suited to solving multidimensional equations if they are properly arranged.

CONCLUSIONS AND RECOMMENDATIONS

It is essential that the staff have modeling capability for studying the phenomena of heat, mass, and eventually solute transport is unsaturated media. The TOUGH code appears to be worthy of our continued support. The efforts currently underway or contemplated under our Research and Technical Assistance contracts with SNL should continue. The following tasks should be pursued under these contracts:

1. Document the code. Provide a user's guide and self-teaching curriculum. These tasks are contemplated under FIN-A1158.

2. Validate and verify the code. These tasks are contemplated primarily under FIN-A1166, but will also come under FIN-A1158 and FIN-A1266.

3. Improve stability and efficiency of code. In this regard:

   a. explore a simpler and more efficient scheme for arranging and numbering elements that takes advantage of banded matrices.

   b. look into more efficient algorithms (e.g., Co83).

   c. Rearrange coding to take advantage of vector-solving ability of the CRAY-1.

These tasks are contemplated under FIN A1266.

The TOUGH code will be a worthwhile addition to the WMGT code arsenal, and will allow the staff to check on the computations on the NNWSI repository performed by or for DOE.

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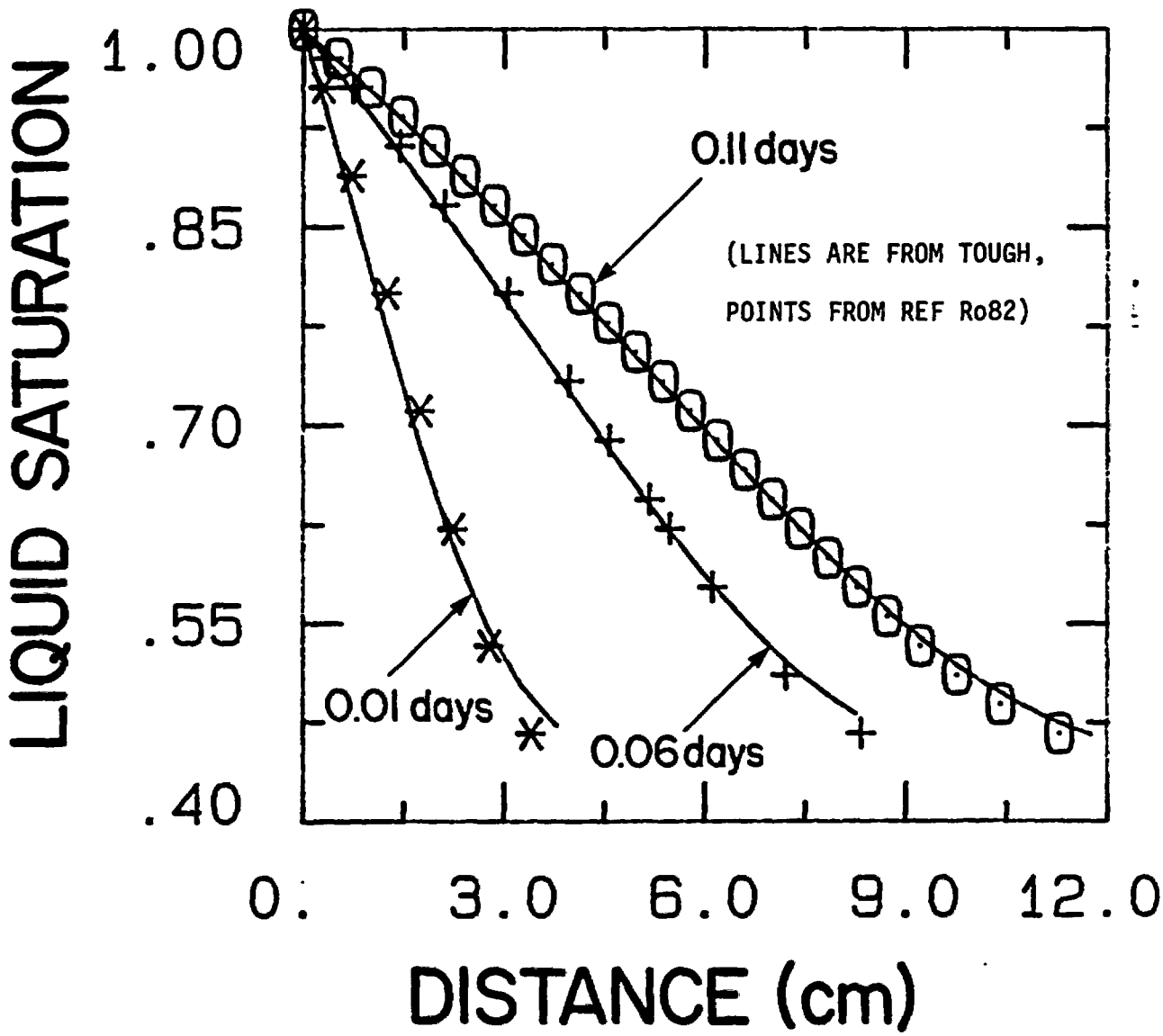

FIGURE 1 - TOUGH SOLUTION FOR PHILIP PROBLEM XBL 836-287

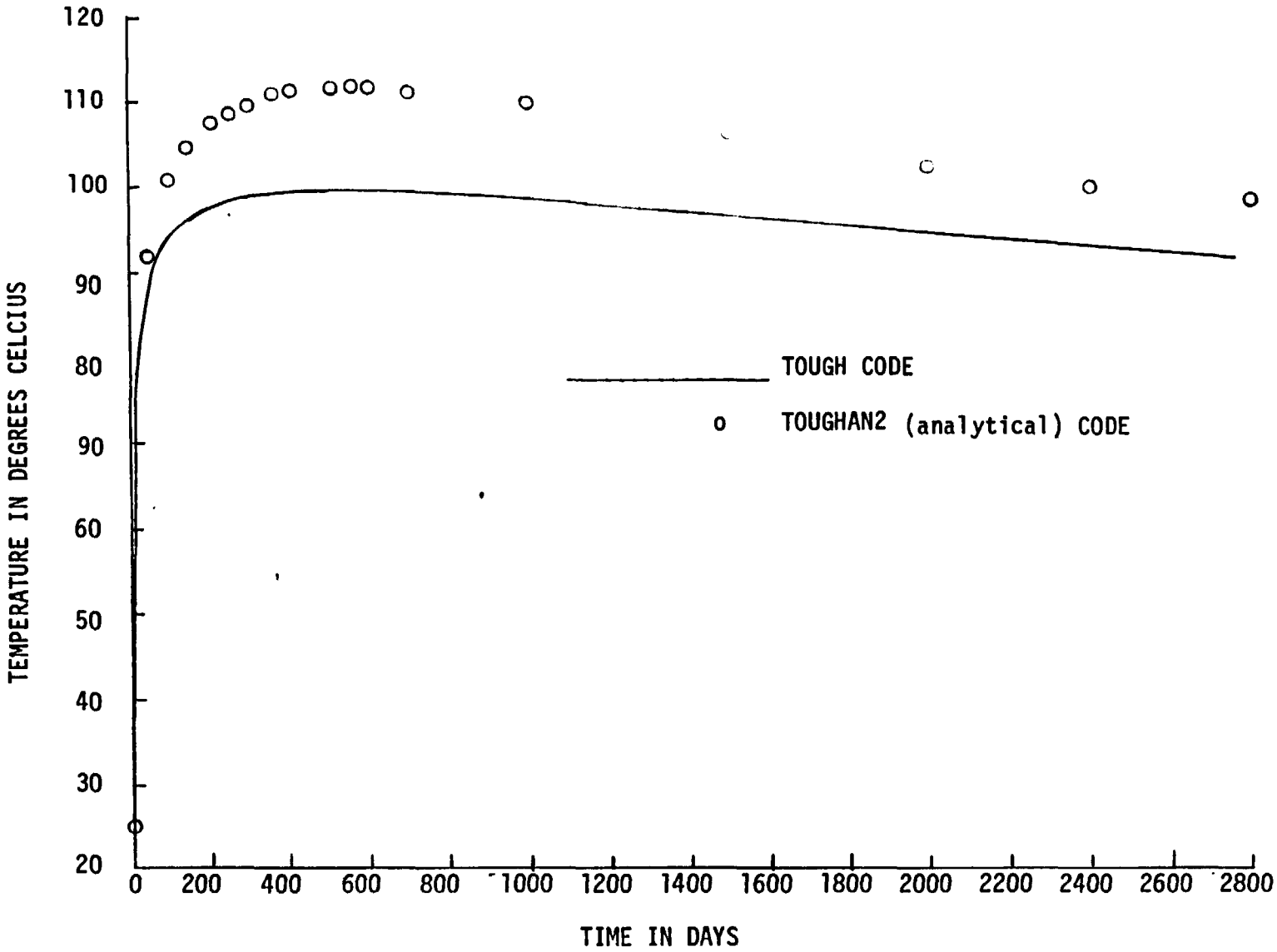

FIGURE 2 - TEMPERATURE HISTORY IN CENTER OF CANISTER

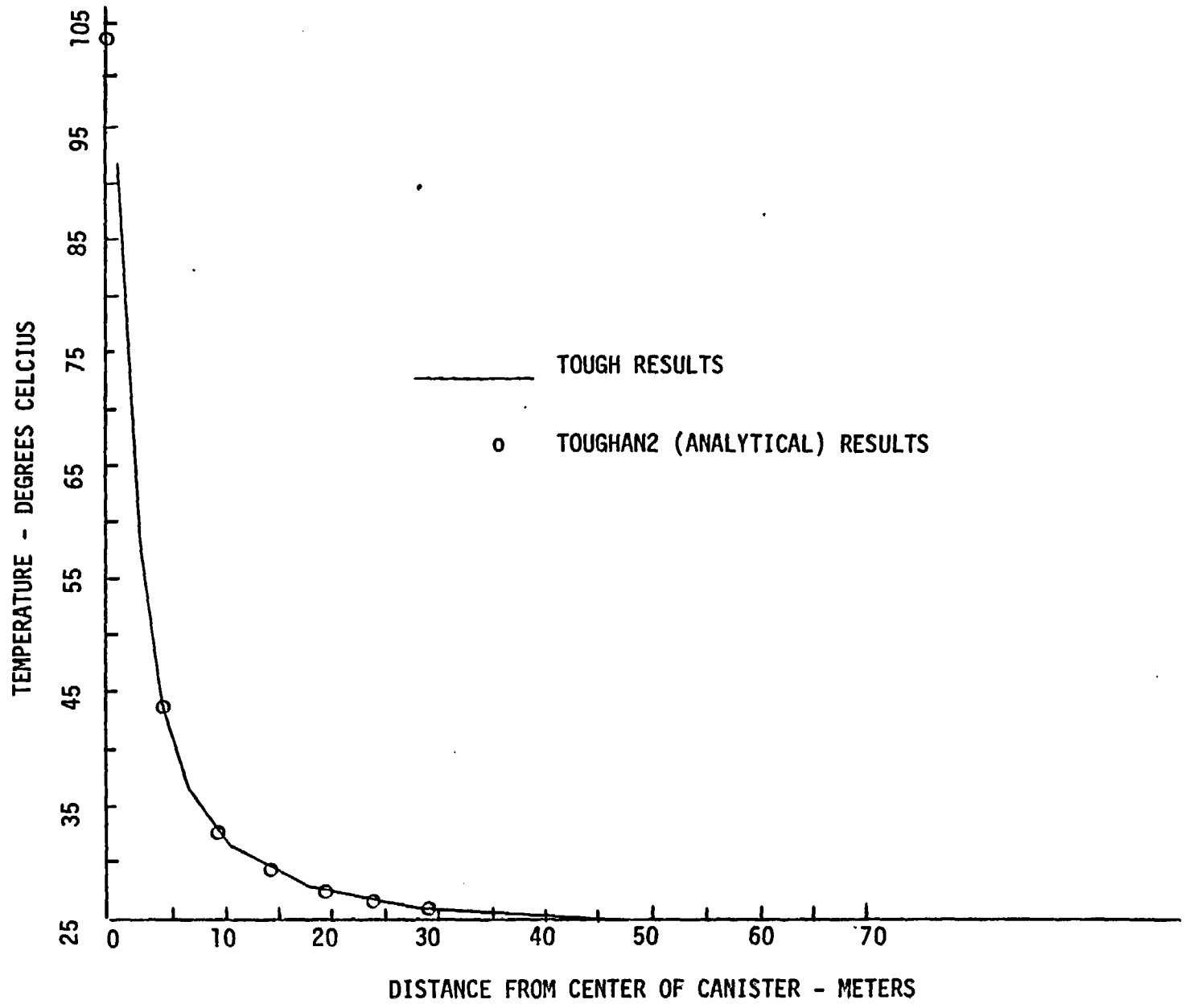

FIGURE 3 - HORIZONTAL TEMPERATURE PROFILE FOR CANISTER A 2767 DAYS

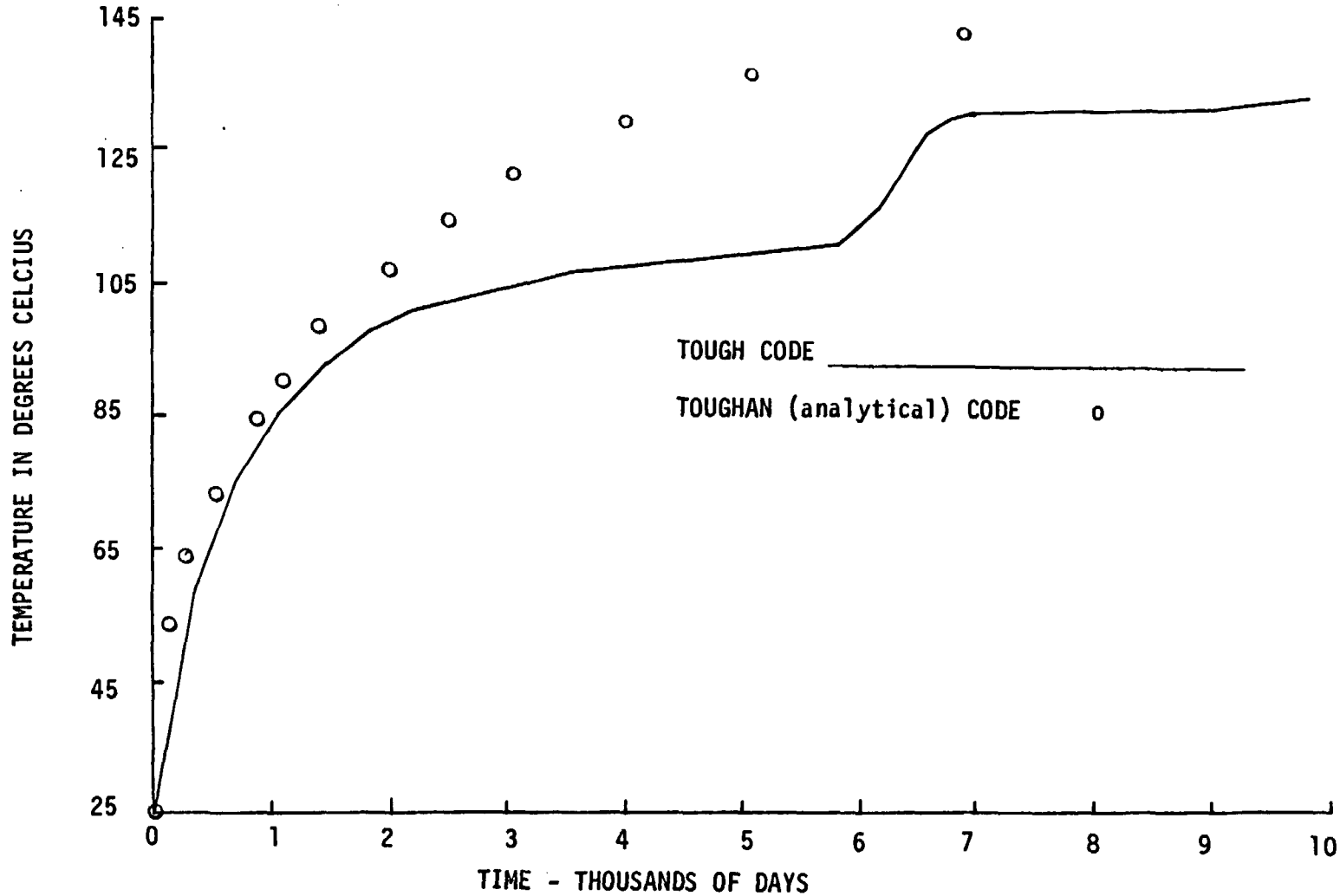

FIGURE 4 - TEMPERATURE HISTORY AT CENTER OF REPOSITORY

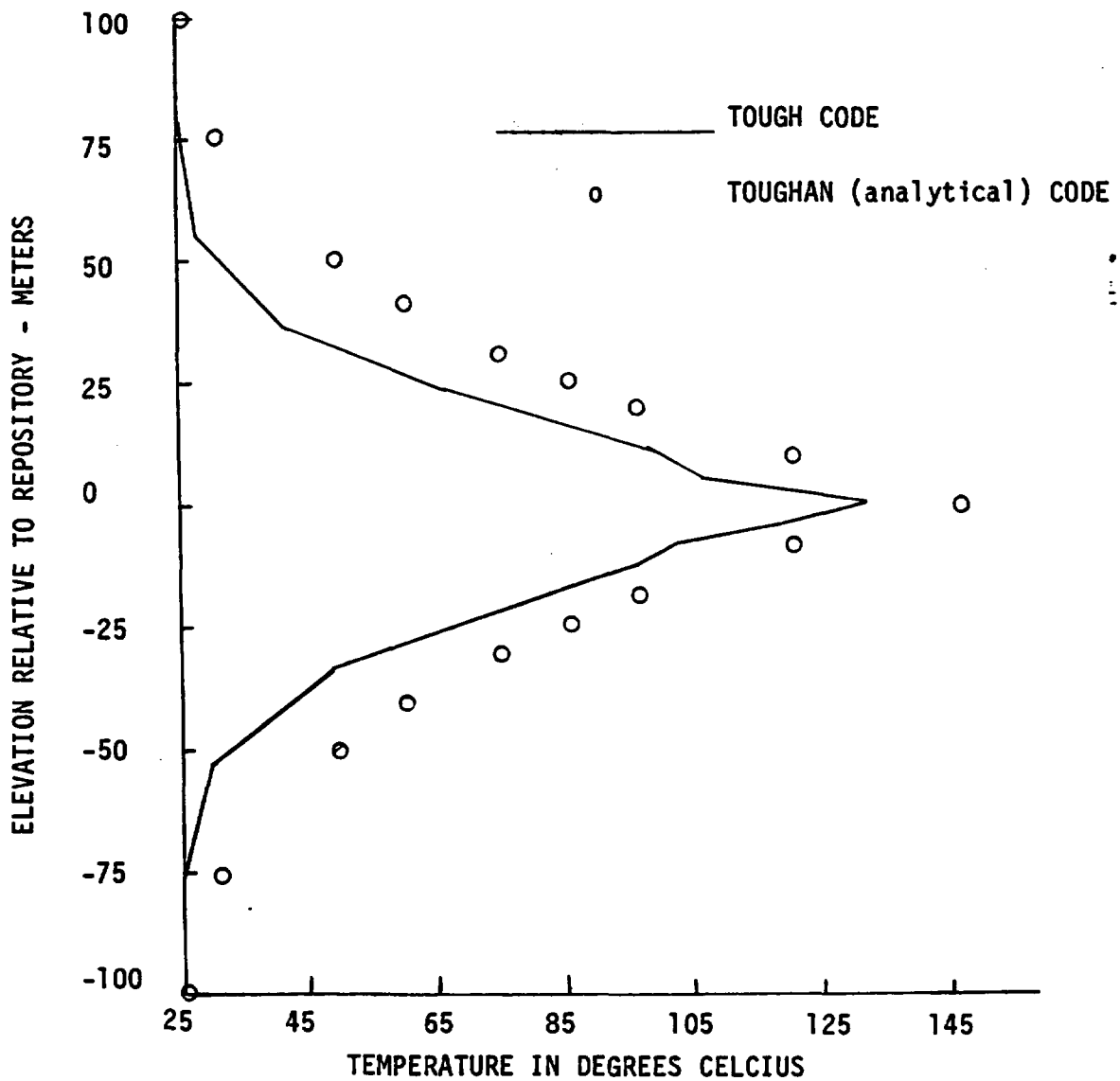

FIGURE 5 - TEMPERATURE PROFILE THROUGH CENTER OF REPOSITORY (R = 0)