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MEMORANDUM FOR: File 3109.9 FEB 16 1984

FROM: M. J. Wise
Repository Projects Branch
Division of Waste Management

SUBJECT: REVIEW OF NWFT/DVM GRAPHICS PACKAGE

Attached is a report written by John Fields, a summer intern in the WMHL branch during the summer of 1983. The report summarizes the effects of two changes (different random number generator and hardwired travel time) on the output of the NWFT/DVM graphics package.

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M. J. Wise
Repository Projects Branch
Division of Waste Management

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WASHINGTON, D. C. 20555

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REVIEW OF NWFT/DVM GRAPHICS PACKAGE

This report is a summary of an investigation into the NWFT/DVM graphics package (UNCLE). Through running the package, several inconsistencies in the output became apparent. These inconsistencies were investigated and the results are documented here.

I. INTRODUCTION

NWFT/DVM is a quasi-two dimensional flow and transport code which has been modified to employ the Latin Hypercube Sampling technique. Variables such as conductivity, elemental solubility, and porosity are assigned ranges and probabilistic distributions from which the Latin Hypercube makes selections. This selection process is done by means of a random number generator (scrambler) that determines the combination of selected parameter values. The scrambler is sixteen numbers, each ranging in value from zero to seven, and arbitrarily chosen by the user.

The input deck contains twenty six variables that are given ranges and probabilistic distributions. The input deck also assigns constant values to many other parameters as well. Flow path, length of flow path, area of flow path, isotopes, and elevations are examples of the constant values. Each of the variables is incorporated into 2200 separate runs. The package then produces output in graphical format. The programs used for this report are stored in the Brookhaven Computer Facility under the names FIELDSWTZEO and FIELDSHWLT using the ID=WISE.

Some of the graphics terminology should also be explained. Travel time is groundwater travel time, average value is the summing and averaging of a function through a range and dividing by the EPA Standard value. Probability is the probability of exceeding the EPA Standard.* Total Disch/EPA is the total discharge divided by the EPA Standard. Release Rate is the rate at which radionuclides are released from the waste package and become available for transport. EPA Ratio is the total release divided by the EPA Standard. Unrestricted is all 2200 runs, as opposed to, for example, only those runs that exceed the EPA Standard.

II. LATIN HYPERCUBE SCRAMBLER

The first series of tests performed on NWFT/DVM used the permanent file FIELDSWTZEO. These tests were basically on the Latin Hypercube. Simply by changing the scrambler used by Latin Hypercube to pick its values,

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* except where indicated.

differences in the graphs occurred. These differences could be anticipated because of the nature and scale of the ranges. Figure 1 shows no discharge of any material for groundwater travel times less than 250 years nor is there any discharge for groundwater travel times between 400 and 1000 years. Figure 2 apparently shows no discharge for groundwater travel times of less than 400 years. These "holes" in the graphs occur because there is not enough data at those points to plot on the graph. While the general shapes of the curves are similar, their values are very different. For instance in Figure 1, at a travel time of 1000 years, the value of the function Total Discharge/EPA has a value of a little over 1. While in Figure 2, at the same point, the Total Discharge/EPA function has a value of .15. This means that the average value of the function Total Discharge at a groundwater travel time of 1000 years in Figure 1 is approximately the EPA Standard. However, in Figure 2, the same point is only 15% of the EPA Standard.

These results highlight the limitations of this type of analysis. The analysis may not be used to evaluate a specific site. However, the probabilistic nature of the analysis is ideal for investigating the relative importance of particular variables. For example, in both Figures 1 and 2, it can be seen that Tc99 is an important contributor. Similarly, for Release Rates, the different scrambler can change the results dramatically as shown in Figure 3 (original scramble) and Figure 4 (new scramble). These results are caused by a lack of data but instead of getting "holes" in the graph, the average value of the function is made extremely low causing Figure 4 to have such drastic fluctuations.

III. HARDWIRING IN AVERAGE VALUE PLOTS

This problem of "holes" in the graphs was solved by using a hardwired approach to the travel time. Hardwiring means that the variable (there are three options: canister life, leach time, travel time) may be assigned a certain range of values that it may have. The difference between hardwiring travel time and release rate is a very significant one. When release rate is hardwired, it is hardwired for a range of values (10^{-7} to 10^{-3}). For these runs, this range coincides with the range that Latin Hypercube assigns to release rate. However, when hardwiring is placed on travel time it is given a range of 100 to 10,000 years. Whereas, when travel time is not hardwired, it is a calculated value and no range is assigned at all. This is explained further in Section V. When hardwired, this range is split up into a number of intervals (also specified by the user) for which a certain number of runs are assigned. In Figure 5 travel time has been hardwired to 11 values between 100 and 10,000 years. The hardwiring tests were performed using permanent file FIELDSHWLT. When comparing the average value plots of Figures 5 and 6 one notices the effects of hardwiring right away. Notice that the Total Disch/EPA points are very similar but there are many holes that hardwiring has filled in. However, hardwiring does affect the values that are calculated. One such point of interest is travel time of 100 years where the hardwired curve moves downward from a point approximately 5.5 times the EPA Standard, and the non-hardwired curve moves upward from approximately 1.1 times the EPA Standard. However the rest of Figure 6 is too full of "holes" to see clearly any other differences but it does appear similar to Figure 5. The reason for all these "holes" is that there were not many runs that satisfied the graph conditions in the first place.

In contrast to the Groundwater Travel Time plots, the Release Rate graphs show a remarkable likeness to one another. The shapes of the Total Discharge curves in Figures 7 and 8 are almost identical. However it is disturbing that the values of the curves vary by approximately an order of magnitude, the hardwired curve being the lesser value. The reason for this wide difference can be explained using Figures 17 and 18. These figures give the probability of the Total Discharge/EPA function being greater than the value shown on the horizontal axis. In Figure 17 approximately 30% of the runs have a Total Discharge/EPA value of greater than 1, or 30% of the runs exceed the EPA Standard. While in Figure 18, only 25% of the runs exceed the EPA Standard. However when one looks at 10 times the EPA Standard, barely 1% of the runs in Figure 17 exceed that limit. While in Figure 18, 10% of the runs exceed 10 times the EPA Standard. In fact, 4% of the runs in Figure 18 exceed 100 times the EPA Standard and approximately 1% exceed 1000 times the EPA Standard. This is important because Figures 7 and 8 are plotting the average values of the Total Discharge/EPA function. Even though Figure 18 shows that only 25% of the runs are greater than the EPA Standard, many of those runs exceed the EPA Standard by a factor of 10 and even 100. So naturally the non-hardwired average values should be greater in Figure 8.

IV. HARDWIRING IN SINGLE VARIABLE DEPENDENCE PLOTS

Thus far all the plots that have been looked at have been average value plots. The graphics package also performs single variable dependence plots. These plots are based on the probability of a subset being in a function. In other words, the probability, in this case (Figures 9 and 10), is the probability of the runs at a specific release rate exceeding an EPA ratio of 1, that is, the probability of exceeding the EPA Standard. So at a release rate of .001 the probability of exceeding the EPA Standard drops from 90% in hardwired to 50% in non-hardwired, a significant decrease. The reason for this drastic change may be explained by using Figures 15 and 16. In Figure 15 no runs exceed a travel time of 10,000 years, while in Figure 16, 50% of the runs exceed 10,000 years of travel time. For those runs which have a travel time of greater than 10,000 years,there are no releases during the period of interest, and therefore, those runs do not exceed the EPA Standard. So when Figure 9 is calculating those runs that exceed the EPA Ratio, no particular run meets the standard simply by having a travel time greater than 10,000 years.

However, for the non-hardwired case, Figure 10 shows that approximately 50% of the runs meet the standard by having travel times greater than 10,000 years. Of the 50% of runs which were not excluded due to travel times greater than 10,000 years, nearly all of those runs exceeded the EPA Standard. This is shown on Figure 10 at the release rate of 10^{-3}, approximately 50% of the runs exceed the EPA Standard. However, 50% of the total runs had been excluded because of Travel Time considerations.

This is in contrast to Figures 11 and 12 which are based on the probability of runs at a specific travel time exceeding the EPA Standard. There is little difference in these graphs except for the fact that Figure 11 drops to zero in several places due to a lack of data points.

V. HARDWIRING IN CCDF PLOTS

Another type of plot generated by NWFT/DVM is a CCDF plot (Complementary Cumulative Distribution Function). These graphs plot the probability of meeting or exceeding the value shown on the horizontal axis. So when the function on the horizontal axis is hardwired a step function should occur. When a particular variable is hardwired, the code assigns the function a particular value for an interval. So, the range will be divided into the specified number of intervals and the endpoints of the range will be initialized to probabilities of one and zero. This can be clearly shown in Figures 13 and 14. Notice that although Figure 14 is not hardwired it does match up very well with the hardwired version. This would seem to indicate that the Release Rate function is not affected significantly by the hardwiring feature. This is because, in these runs, the range of its values is the same whether it is hardwired or not, and only the number of intervals varies. In contrast to this, the groundwater travel time is very distorted as shown in Figures 15 and 16. The hardwiring again gives an even step function beginning at a travel time of 100 years and ending at a travel time of 10,000 years. This means that all the runs are greater than or equal to a travel time of 100 years and none of the runs exceeds a travel time of 10,000 years. If travel time is not hardwired, the program calculates that 20% of the runs have travel times of less than 100 years and about 47% have travel times greater than 10,000 years.

V. RESULTS OF FINDINGS

An explanation for the difference in groundwater travel time distribution between hardwiring and non-hardwiring goes back to the equation for groundwater travel time.

TT = Ld/Ki

L = length of flow path

d = effective porosity

K = hydraulic conductivity

i = hydraulic gradient

Each of these variables are defined in the input deck of the program. Conductivity, porosity and hydraulic gradient are all values that are picked from a designated range by the Latin Hypercube Sampler. The length of flow path is a constant value. When travel time is not hardwired, the Latin Hypercube picks all other values at random and travel time is calculated. When the travel time is hardwired a certain number of runs is designated for each interval. Therefore a travel time is already picked by the program and some other parameter must be varied. At this point the program works backward from the non-hardwired version. The program has a travel time and calculates a conductivity. Since the conductivity may jump several orders of magnitude due to this hardwiring the overall results are affected.

VI. CONCLUSION

The NWFT/DVM graphics package provides valuable insight into the relative importance of particular variables. However, as shown in this report, the user must exercise caution when using the package. Often it may be necessary to look at several graphs to understand the impact of one variable. This is particularly true when interpreting average value plots.

The hardwiring feature of the package guarantees that the intervals of interest will contain enough points to eliminate the "holes" that sometimes appear. That is, the travel time hardwiring forces all runs to remain within the 10,000 year period. Two cautionary notes are necessary. First, although this technique fills the "holes", it also may be misleading. By forcing all runs to have travel times less than 10,000 years, a significant percentage of the runs that would have met the EPA standard (automatically) are eliminated. Second the user should be aware of the hydraulic conductivity "refit" that occurs when travel time is hardwired. Also, this "refit" is not reflected in the single variable dependence plots using conductivity as the variable. In other words, for these plots, the package uses the conductivity values chosen originally by the LHS code, and not the "refit" values.

Finally, when the graphs are to be used for comparison purposes, it is important that the same scrambler be used. As shown earlier, a change in the scrambler can have a dramatic effect on the numerical results, although the shape of the curve is not substantially affected.

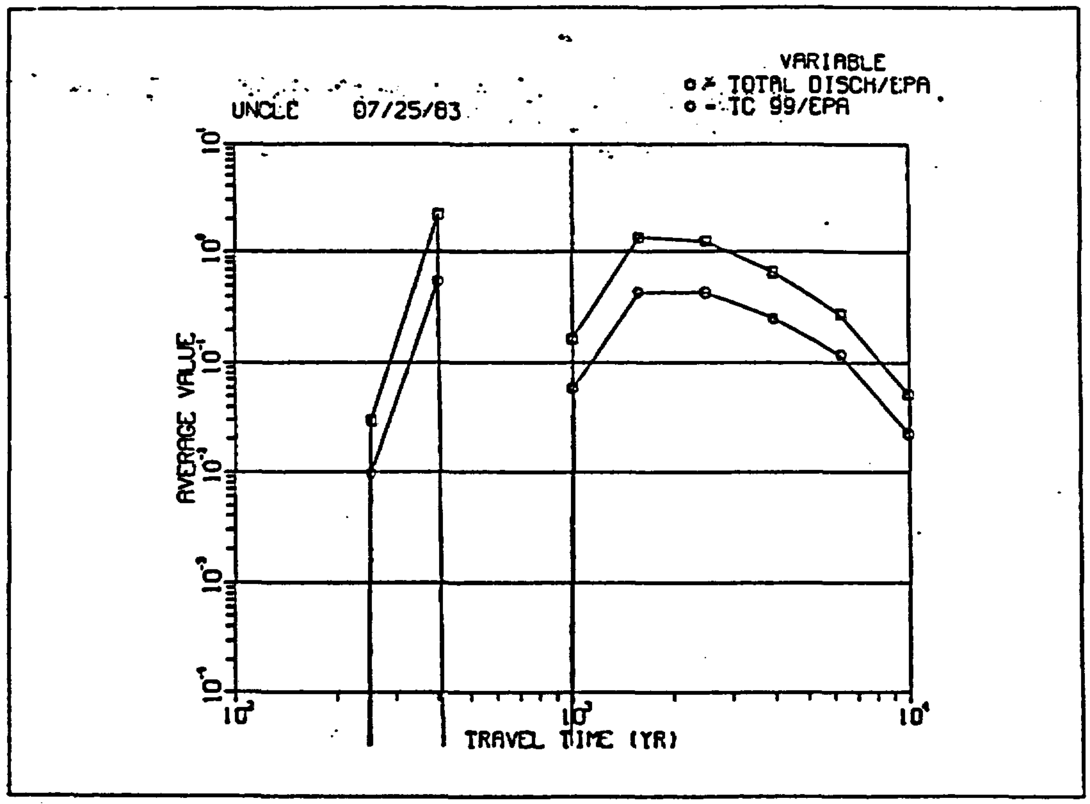

Figure 1. Regular Scramble.

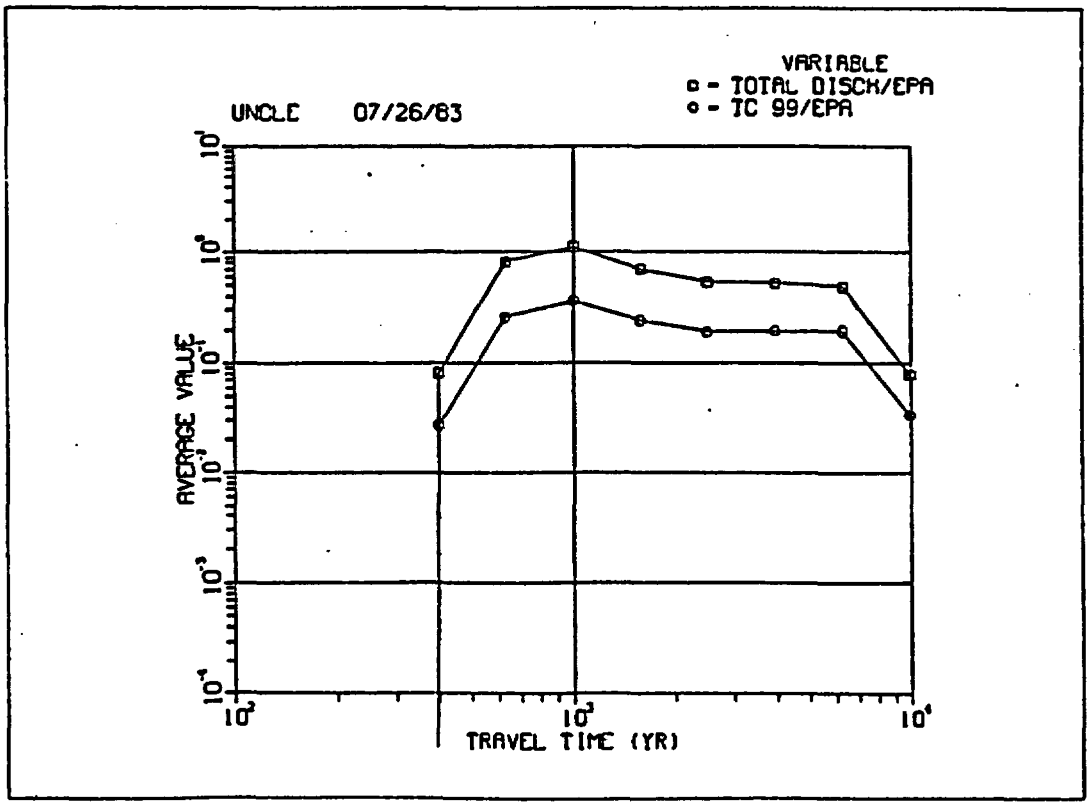

Figure 2. New Scramble.

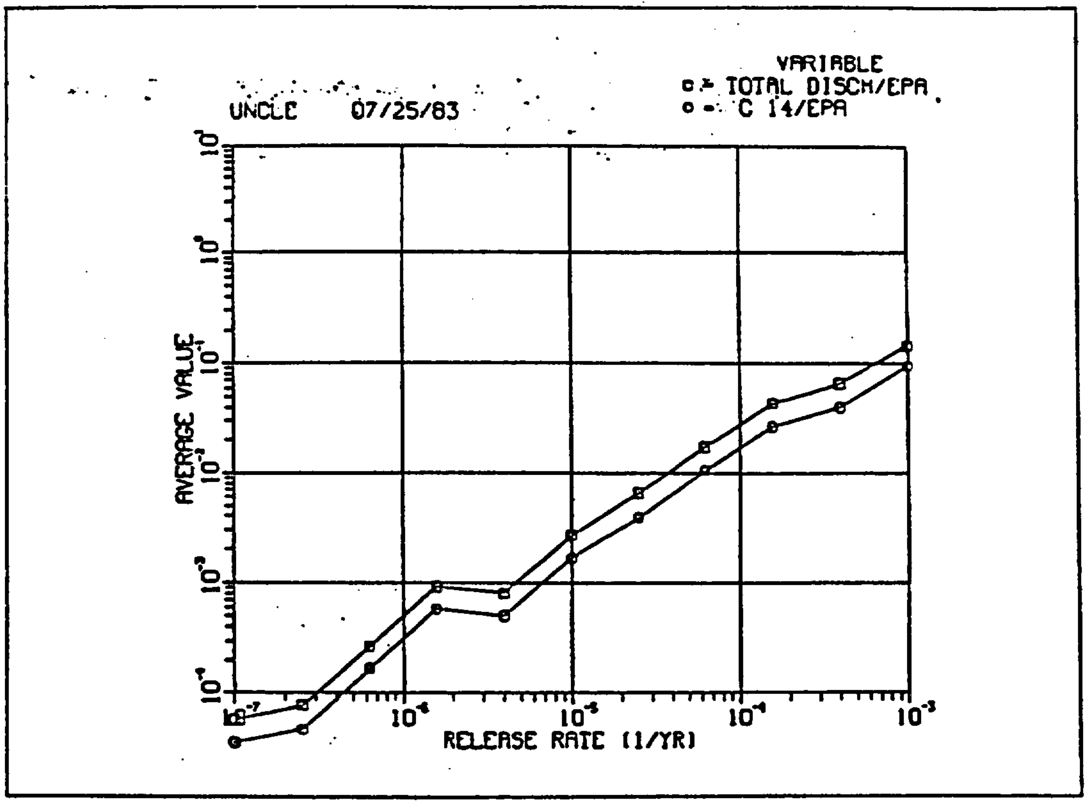

Figure 3. Regular Scramble.

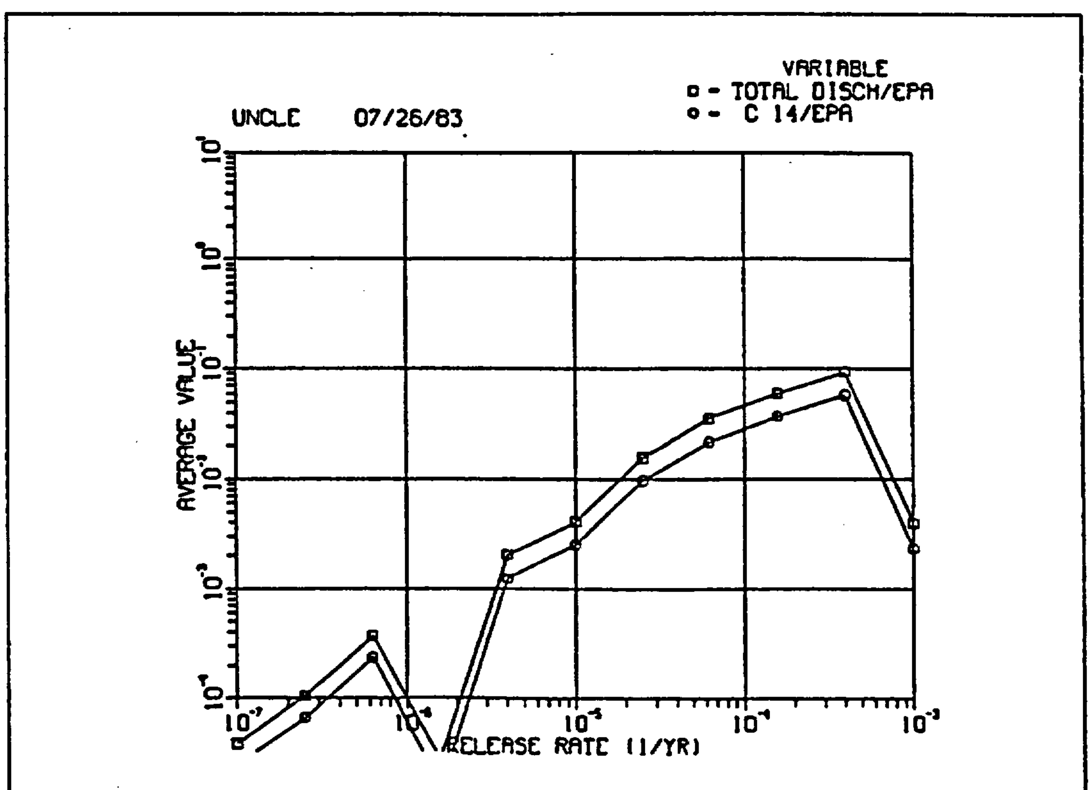

Figure 4. New Scramble.

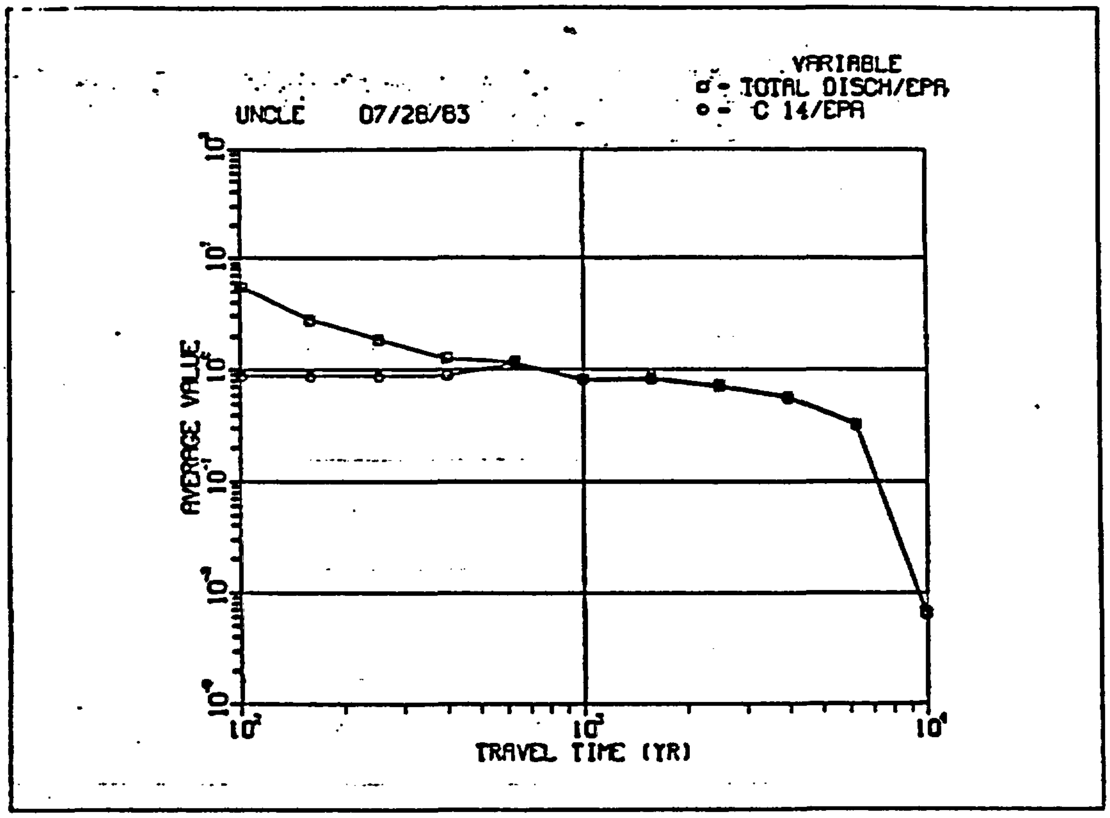

Figure 5. Hardwired Travel Time.

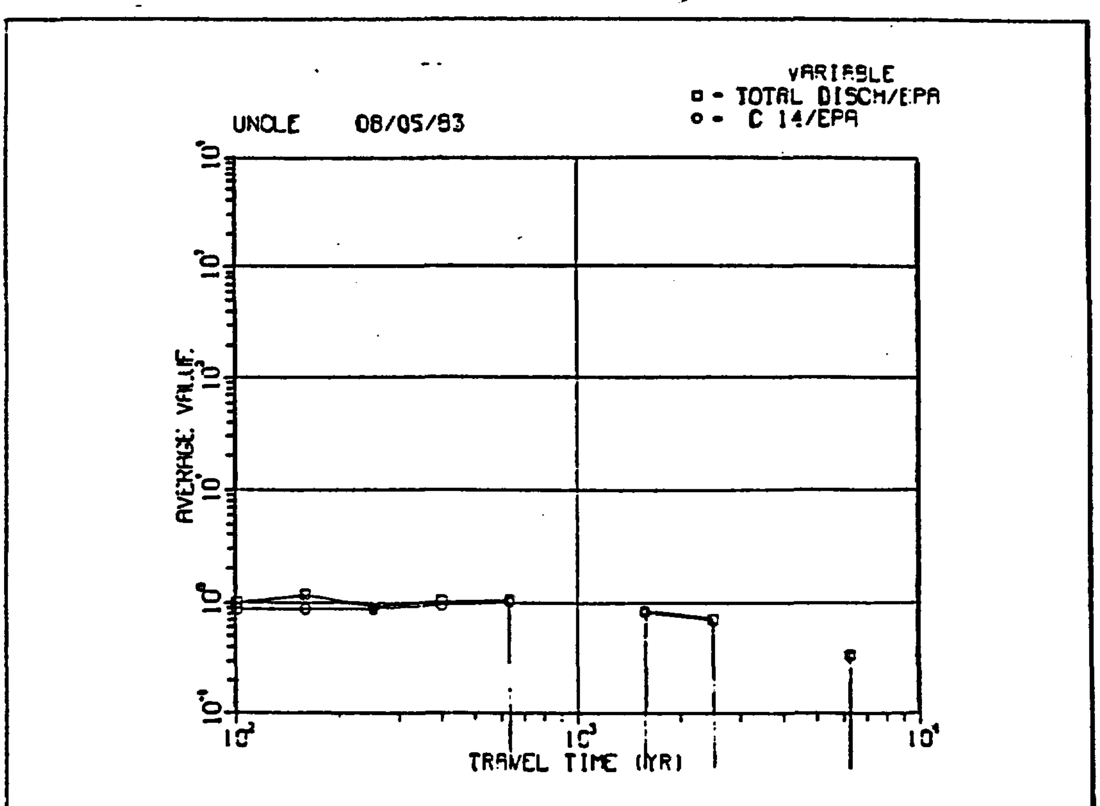

Figure 6. Non-Hardwired Travel Time.

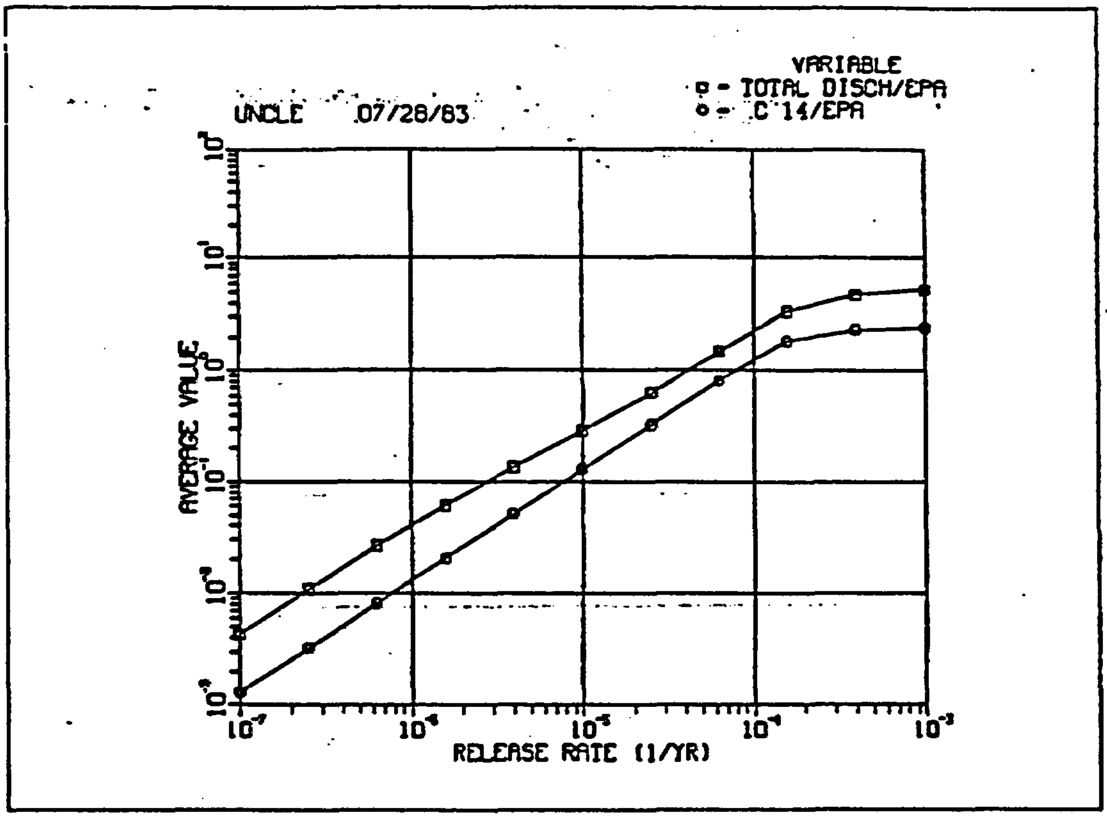

Figure 7. Hardwired Travel Time.

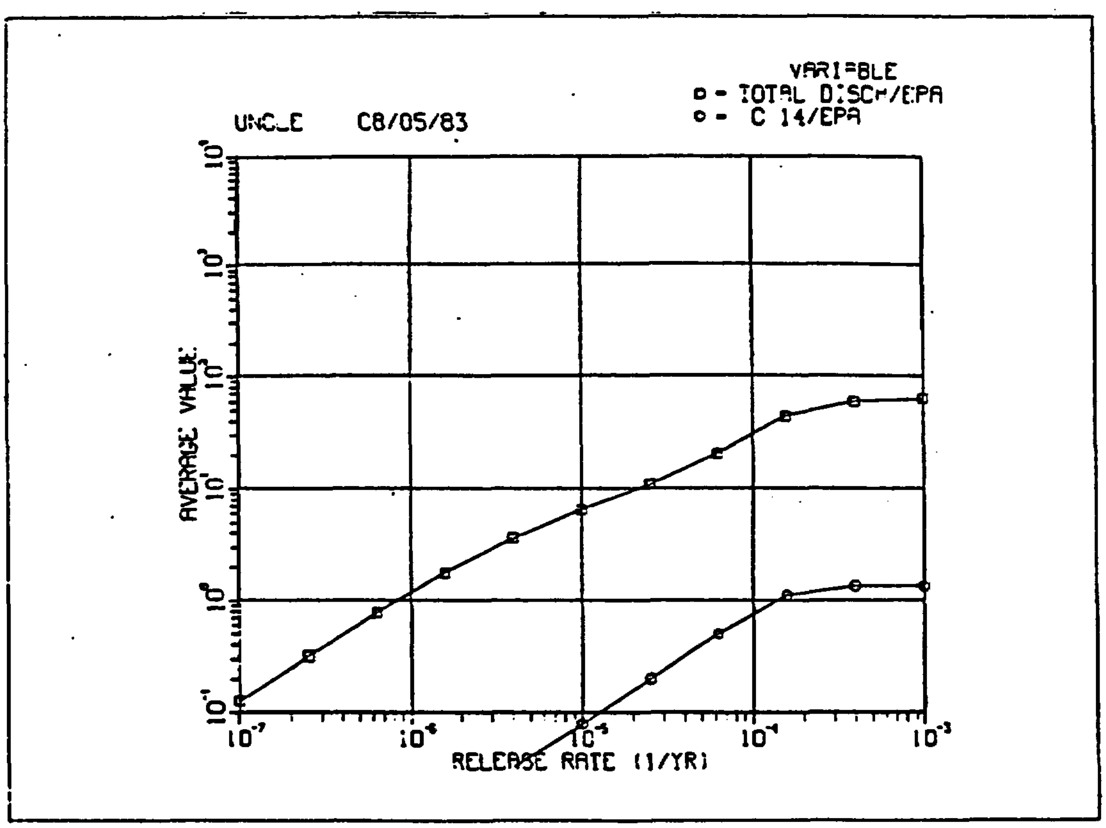

Figure 8. Non-Hardwired Travel Time.

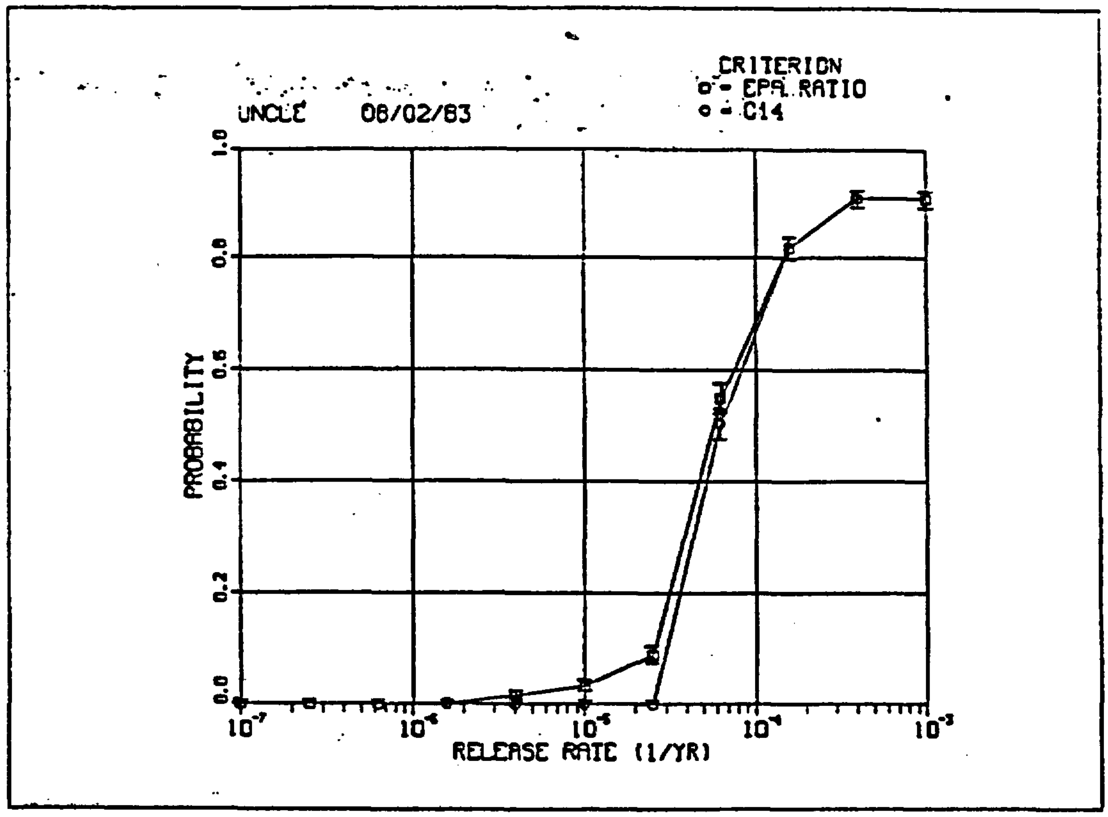

Figure 9. Hardwired Travel Time.

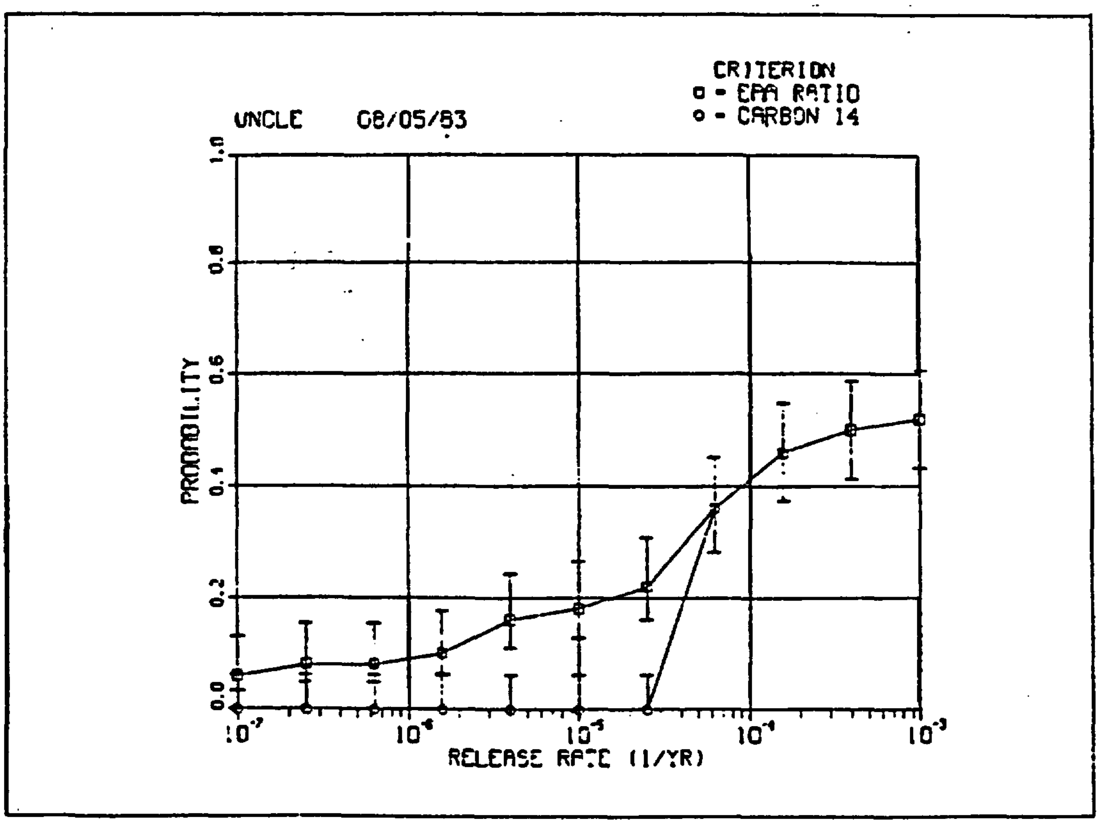

Figure 10. Non-Hardwired Travel Time.

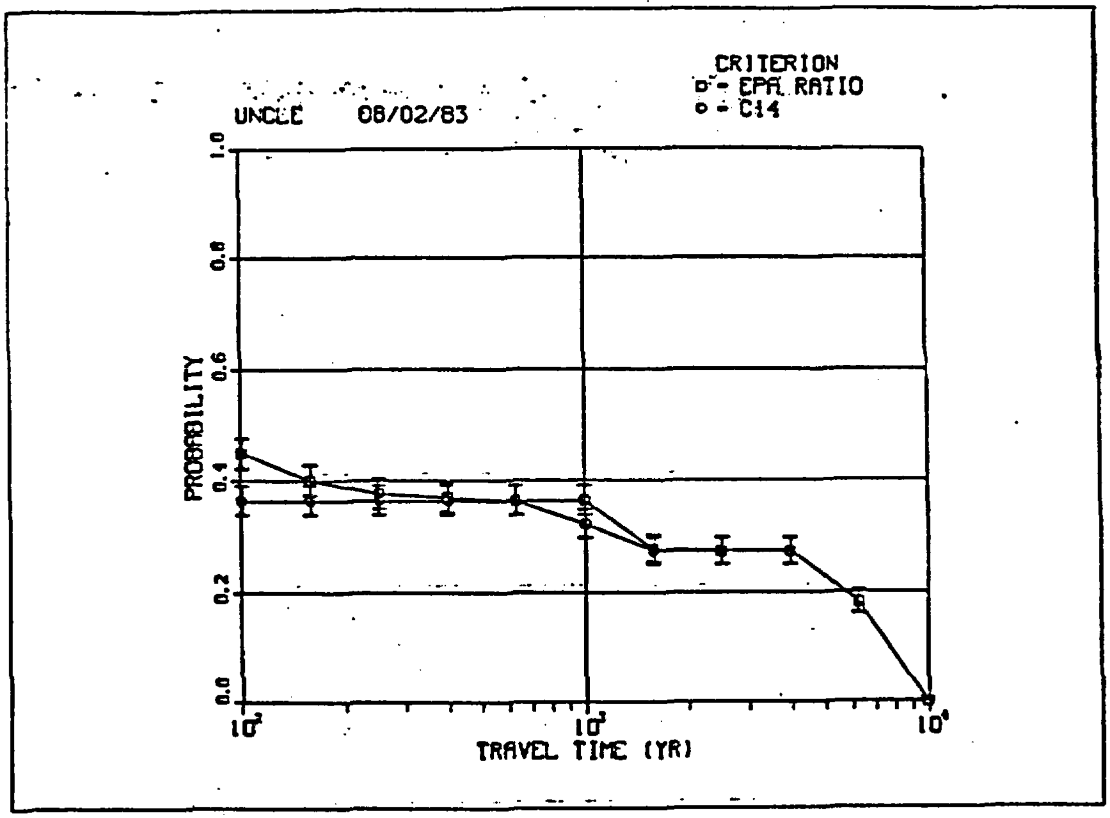

Figure 11. Hardwired Travel Time.

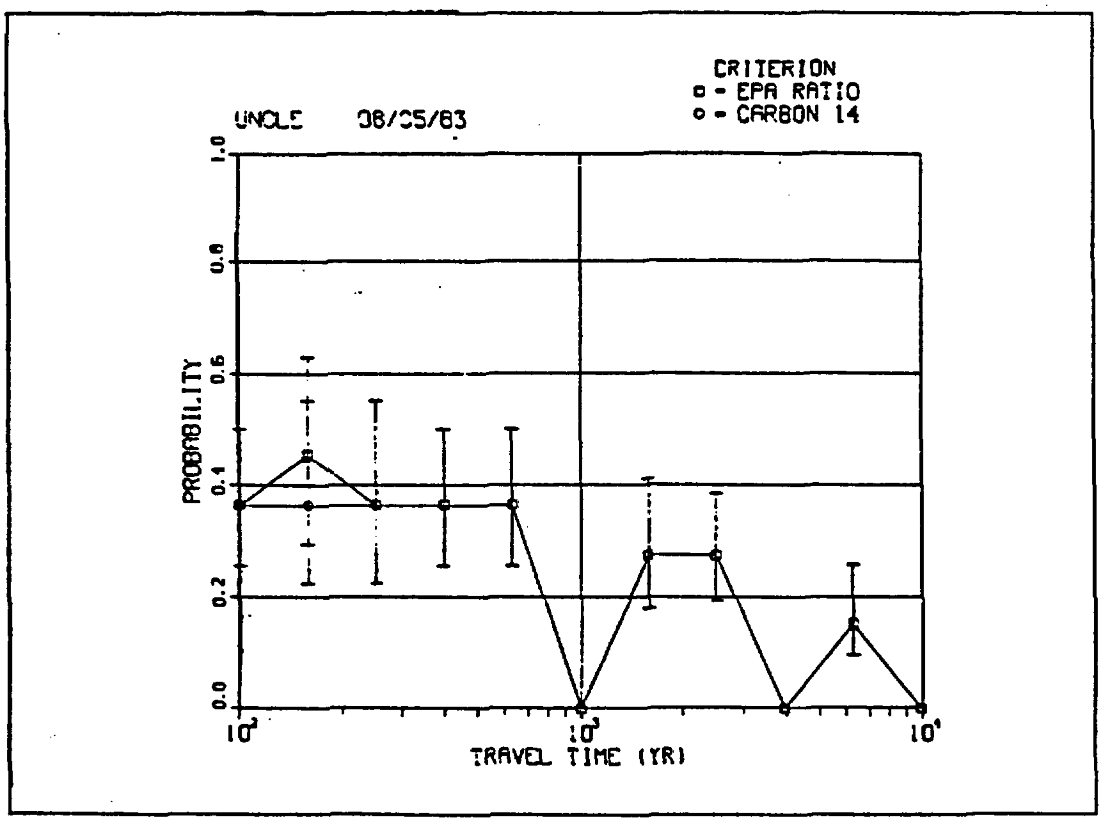

Figure 12. Non-Hardwired Travel Time.

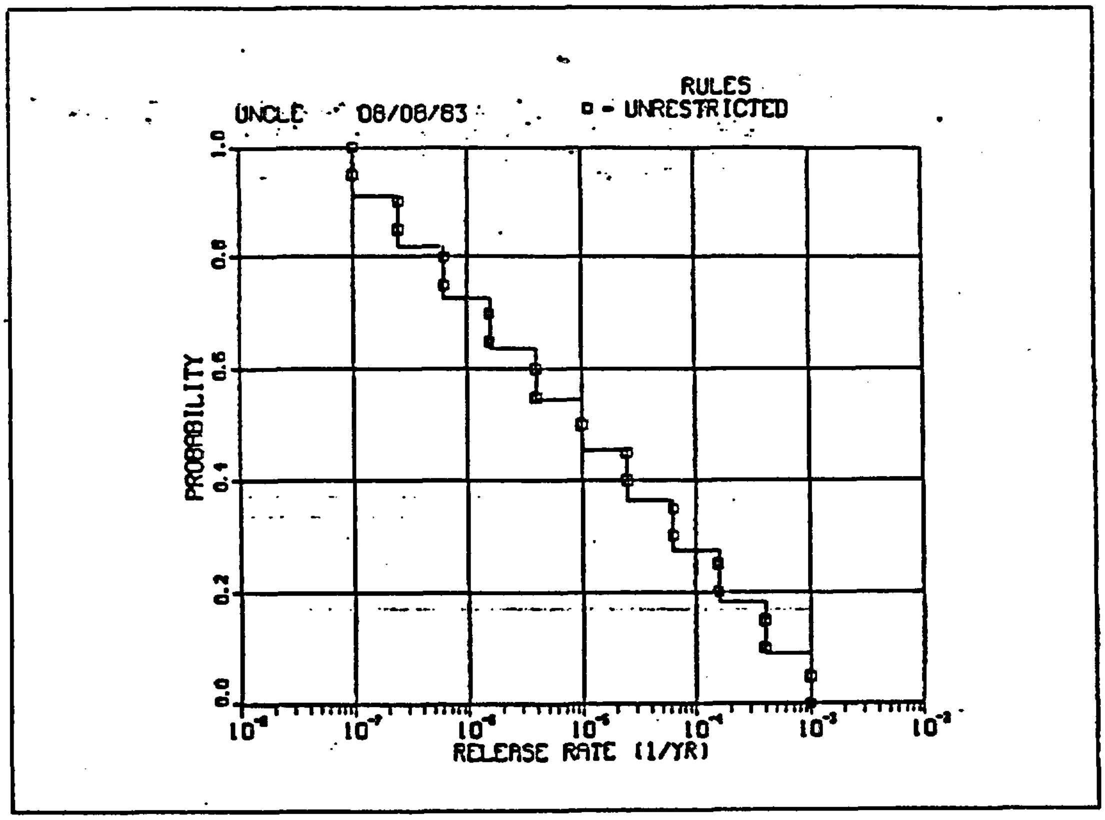

Figure 13. Hardwired Release Rate.

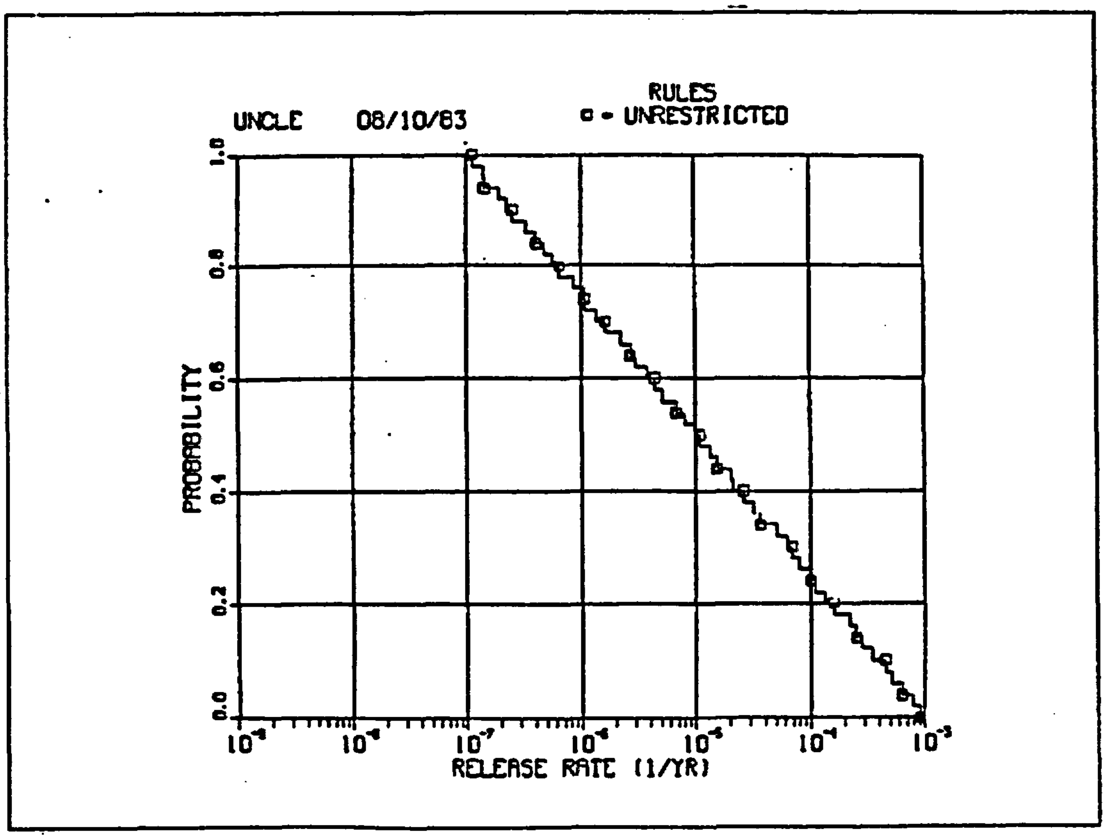

Figure 14. Non-Hardwired Release Rate.

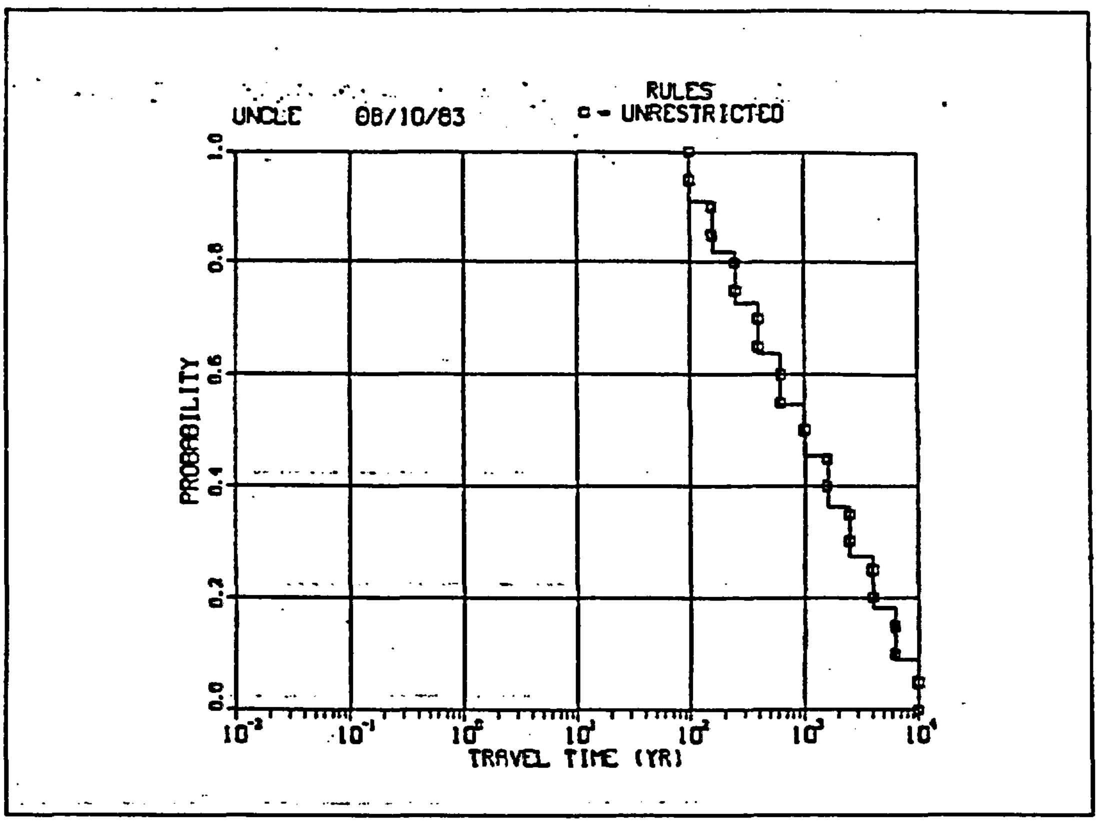

Figure 15. Hardwired Travel Time.

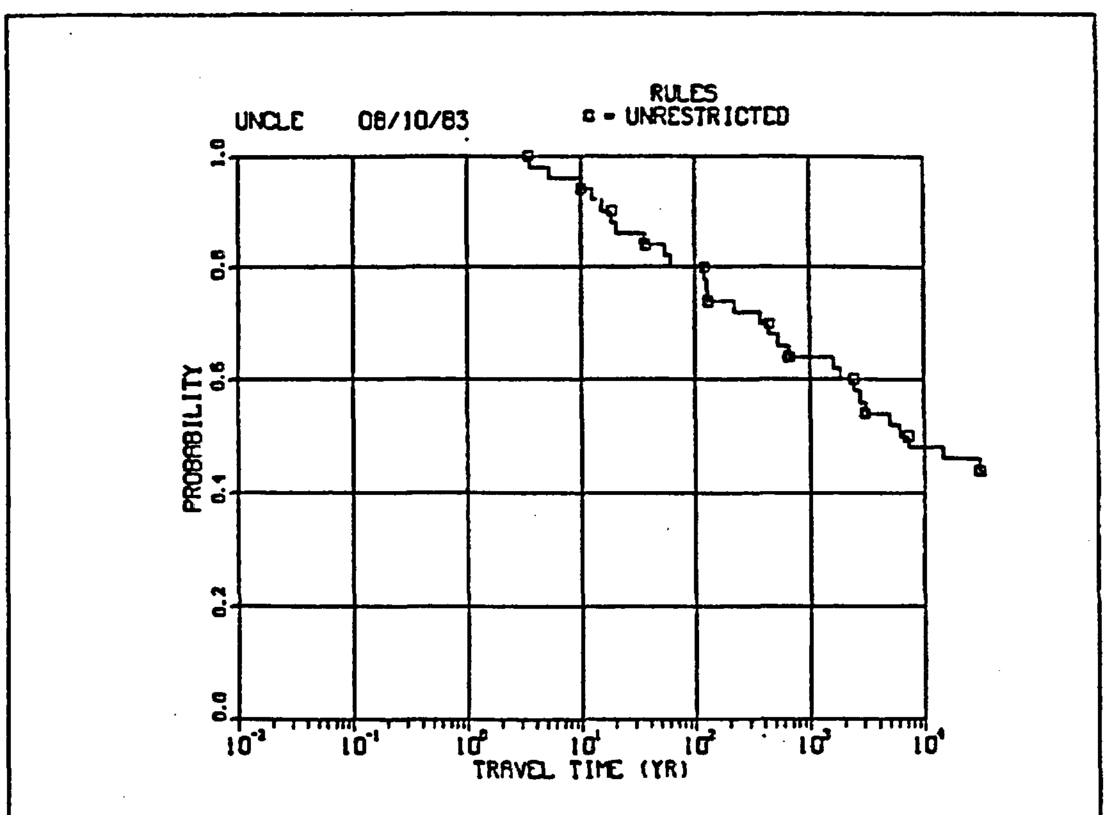

Figure 16. Non-Hardwired Travel Time.

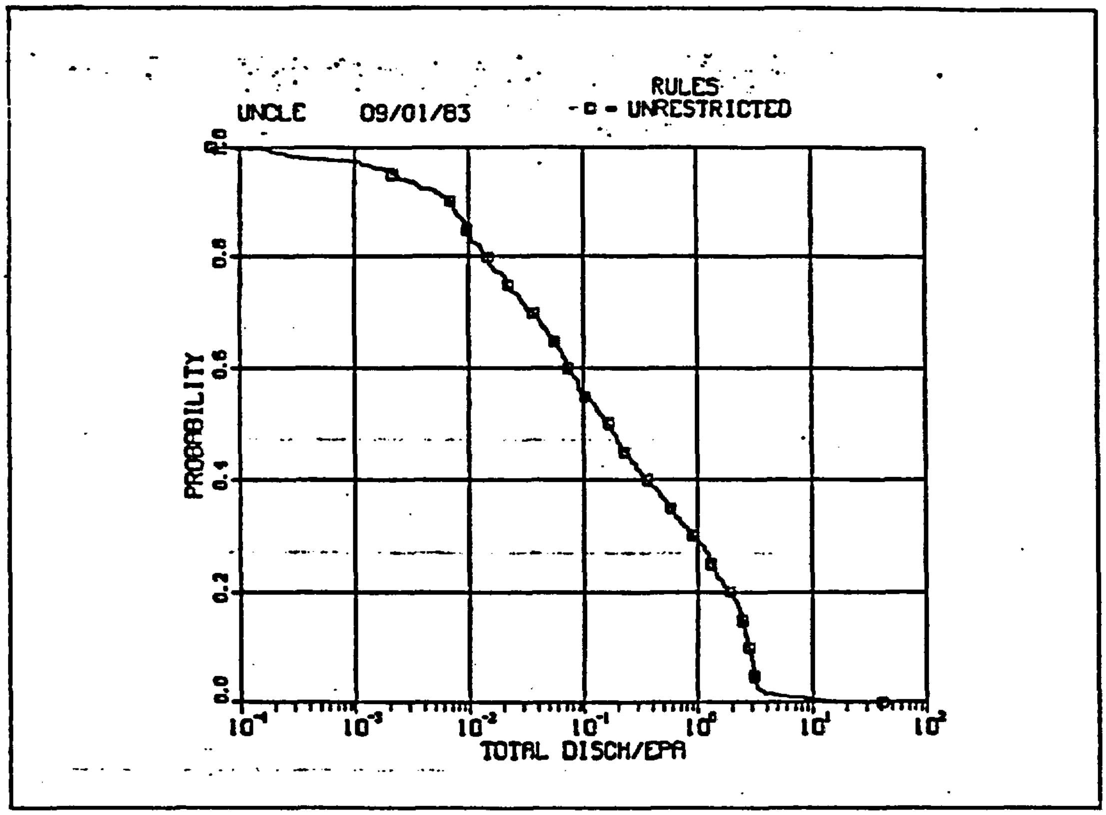

Figure 17. Hardwired Travel Time.

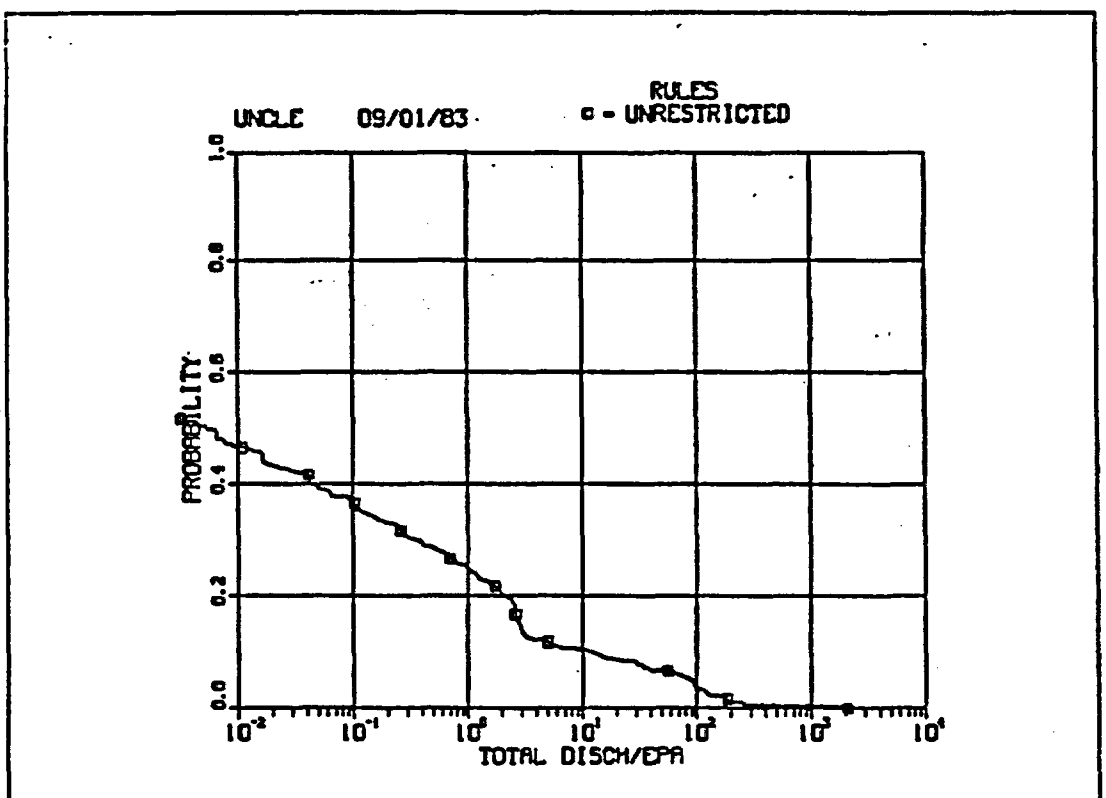

Figure 18. Non-Hardwired Travel Time.