CONF-890855--49

SAND89-1419C

Application of Generic Risk Assessment Software to Radioactive Waste Disposal

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SAND--89-1419C

DE89 013817

* This work was performed at Sandia National Laboratories, which is operated for the U.S. Department of Energy under contract number DE-AC04-76DP00789.

ABSTRACT

Monte Carlo methods are used in a variety of applications such as risk assessment, probabilistic safety assessment, and reliability analysis. While Monte Carlo methods are simple to use, their application can be laborious. A new microcomputer software package has been developed that substantially reduces the effort required to conduct Monte Carlo analyses. The Sensitivity and Uncertainty Analysis Shell (SUNS) is a software shell in the sense that a wide variety of application models can be incorporated into it. SUNS offers several useful features including a menu-driven environment, a flexible input editor, both Monte Carlo and Latin Hypercube sampling, the ability to perform both repeated trials and parametric studies in a single run, and both statistical and graphical output. SUNS also performs all required file management functions.

I. INTRODUCTION

Dramatic advances in computer power and availability in the past few years have been accompanied by a corresponding increase in the use of computer models. In particular, computer models are increasingly used to predict or project the future consequences of current human actions. Examples of such applications include economic analysis, risk assessment, probabilistic safety assessment and product reliability analysis. As more reliance is placed on predictions generated by computer models, there has been a growing awareness of the uncertainties inherent in these predictions. As a result, it has become common to see model predictions presented in statistical terms such as probability distributions or means and variances.

Several methods have evolved in recent years for evaluating model uncertainties. These include adjoint techniques (Chavent 1971 and Sykes, et al., 1985), stochastic methods (Mathis and Wehrly, 1979), Monte Carlo methods (O'Neil, et al., 1981), and perturbation theory (Greenspan, 1976). Certainly Monte Carlo analysis is the most versatile and widely used of these techniques. This paper describes recently developed microcomputer software that considerably simplifies the application of Monte Carlo methods to a variety of problems. The Sensitivity and Uncertainty Analysis Shell (SUNS) was developed to be easily adaptable to almost any problem requiring Monte Carlo analysis. SUNS has been used for hydrocarbon economic analysis, safety analysis for shallow burial of radioactive waste, regulatory analysis of deep disposal of radioactive waste, integrated circuit reliability analysis, and several other applications.

The structure and major features of SUNS are described in Section II and an example application of the software shell is presented in Section III. Section IV provides a summary and conclusions.

II. DESCRIPTION OF SUNS

The SUNS software package has been designed to take advantage of the common features that are part of most studies involving data uncertainties. Figure 1 illustrates the main steps that are typically part of such analyses. The first two steps are to develop or acquire the needed computational capability (i.e., an appropriate computer model), and, based on the modeling approach, to identify the data needed to perform the desired analyses. Data collection is the last step that must be taken before analysis can begin. For analyses that require consideration of data uncertainties, data collection is more than just identifying single values of model input requirements. Model data input that have significant uncertainties must be identified and these uncertainties characterized in the form of appropriate distributions. Data uncertainties may result from measurement error, natural randomness in the physical property represented by the data, or simply from lack of data. In any case, data uncertainties arising from all these sources are typically characterized by assigning distribution functions for model input data.

Another issue involving model data is the possible interdependencies among input variables. If two variables are sampled and their values randomly paired, they tend to be uncorrelated. To account for correlated variables, one can use curve-fitting to describe variable relationships in some best-fit sense or can pair variable values in a structured manner to produce desired statistical correlations. The SUNS package uses the latter approach, which is easily generalized to more than two variables, by linearly correlating the ranks of input variables. Since variables often exhibit monotonic relationships, and since taking ranks of variables transforms monotonic behavior to linear behavior, the use of linear rank correlations has broad application.

Once the modeling capability is in place and input data have been defined, analysis typically follows the remaining steps shown in Figure 1. In conducting studies that involve uncertainty analysis, sampling from input distributions and performing repeated trials is the central focus of the computation. However, it is often useful to conduct parametric studies. Parameter variation studies involve fixing all input variables except one which is then set to a few pre-determined values. In this way, the behavior of model output as a function of individual input variables can be examined. Once output results have been generated and appropriate data files created, results are usually examined using graphics and statistics software.

Performing these several steps may involve as many as four different computer programs; a statistical sampling code, the actual process model being examined, graphics software for plotting results, and a statistical package for examining output statistics.

All the functions shown inside the dashed outline in Figure 1 have been incorporated into the SUNS package. The structure of SUNS is shown in Figure 2.

The primary function of the EXECUTIVE ROUTINE (SUNSEXEC) is to direct program execution to the appropriate module based upon the current status of input and output files and menu options selected by the user. SUNSEXEC performs the major file management functions and provides other utilities such as allowing the user to print the input file or modify the screen colors.

The INPUT EDITOR (SUNSINP) provides a menu driven facility for input file creation and editing. The input prompts and other information presented on the screen substantially reduce the need for user reference to a written software manual. SUNSINP provides cut, copy, and paste capabilities to simplify repetitive input. An example input screen is presented in Figure 3. This screen allows the user to specify variable distributions for certain radionuclide source properties used in the NEFTRAN code (Longsine, et al., 1987) which serves as the example application in the next section. The types of available distributions are listed at the bottom left of the screen.

The STATISTICS DRIVER (see Figure 2) performs the statistical sampling and serves as a driver routine for the user's model. Thus, this software module performs the repeated trials and any parametric analysis requested by the user.

The SUNS POST PROCESSOR provides graphical and statistical output. Graphical output includes histograms, cumulative and complementary cumulative distribution functions, scatter plots, and x-y plots. Statistical output includes minimum and maximum values, means, variances and percentiles. Also available are simple and partial correlation coefficients on both raw and rank data. The user can also directly examine any of the output data blocks. Provision is made for additional hardcopy output to be placed on an auxiliary data output file that can be printed at the user's convenience.

In developing SUNS, the objective was to design a software shell that could accommodate virtually any computer model suitable for use in a Monte Carlo analysis. Accomplishing this objective required more than simply developing the capabilities discussed above. Particular design attention was required for the data input and output interfaces between SUNS and the model to be incorporated into the shell. In developing an input file, a simple line editor could obviously be used for any application. However, the desire was to design an input editor that uses menus and on-screen prompts to simplify input file creation, reduce input errors, and to reduce or eliminate the need to refer to written manuals. To meet this objective, the input editor divides model input into three categories; (1) fixed data, (2) array data, and (3) variable data. In the fixed data category, up to 8 groups of parameters with up to 30 parameters per group are allowed. This category of input is useful for fixed physical properties, run controls, print controls, and other single-valued input. In the array data category, up to 8 arrays (one or two-dimensional) with up to 1000 entries per array are allowed. For the example application presented in the next section, arrays are used to input the initial radionuclide inventory and to provide the geometry and physical properties of the fluid flow network. The last data group, variables, is used for those model inputs that must be treated as uncertain and, therefore, assigned a probability distribution rather than a fixed value. SUNS allows up to 8 groups of variables with up to 30 variables per group. With these input data categories, it has thus far proven straightforward to accommodate a wide range of models into the SUNS shell.

At the output end, the need for generality and flexibility was accomplished by recognizing that the output from most models that might be used in Monte Carlo analysis can be separated into two categories. One category includes results that are used in the form produced by the model. This category might include debug printouts, reflections of input data, etc. The second category consists of output that requires further manipulation to produce graphical or statistical results. The first category of output is accommodated by providing a disk file unit that the application model can write such results to. Results in the second category can generally be cast as rectangular arrays where each column of the array has some common attribute. For example, each trial of a Monte Carlo analysis produces a single record or row of an output array. The first N values in the record are the sampled values of the input variables for that trial. The last M values are the values of the response variables for that trial (SUNS allows up to 30 response variables). Thus, for a statistical output array, the number of columns is N + M and the number of rows is the number of trials. SUNS allows up to 15 output arrays or data blocks to be produced per run. These can be any combination of statistical (results of repeated trials) or non-statistical data blocks. In the application presented below, radionuclide discharge rates as a function of time provide an example of non-statistical output.

Another objective in the design of SUNS was to simplify, to the extent possible, the process of incorporating models into the package. This is accomplished in part by the standardization of information transfer throughout the modules of SUNS. As shown on Figure 4, information is passed between the modules of SUNS using several disk files having the same root name but different extensions. The fact that these files are independent of the user's model means that user involvement in information transfer is restricted to the interaction of SUNS with the user's model, discussed below.

Information is passed to and from the user's model via labeled common. This further simplifies model incorporation by eliminating the need for the user's model to know file structure and format. There are three arrays provided to the user's model, one for parameters, one for arrays, and one for variables. Since SUNS is generic, it has no knowledge of variable names in the user's model. Thus, the user must provide the replacement statements, normally in a subroutine, that equate the model variable names to locations in the three arrays. Typically this routine replaces, and is easier to construct than, a routine that reads model input from an external file. The variable data are provided by SUNS one trial at a time so that replacement statements for variables are accessed on every trial.

Passing results from the user's model back to the STATISTICS DRIVER is also done via labeled common. For statistical blocks this requires a vector of response-variable values for each trail. The complete data block is then assembled by the STATISTICS DRIVER. For nonstatistical blocks the user's model must provide the data block in toto. In either case the STATISTICS DRIVER calculates correlations on both the raw and ranked data for each data block and writes the block and associated correlations to disk file. For a nonstatistical block, correlations are found among all columns of data. For a statistical block, correlations are computed amongst the sampled set of input variables and from each response variable to the set of input variables.

In the post processor (SUNSOUT), all graphics or statistics output is generated by first selecting the desired output data block from a menu, then selecting the desired columns from the output block. For example, to generate simple and partial correlation coefficients for a statistical output block, the user first selects a dependent variable (column) from the response variables. Then up to 15 independent variables are selected from the input variable columns of the output data block. SUNSOUT then calculates and displays the simple and partial correlation coefficients between the dependent variable and the independent variables.

III. SAMPLE APPLICATION

The general risk assessment methodology described above has been applied to the problem of disposal of radioactive wastes in geologic formations. Part of the post-closure analysis involves the potential for wastes to migrate to the accessible environment by natural ground-water convection. Depending on the geology of the disposal site, the events or processes that might allow circulating ground water to contact buried waste are postulated, and are typically called scenarios. The NEFTRAN code (Longsine, et al., 1987) is an efficient simulator for predicting radionuclide discharge given a groundwater release scenario. The incorporation of NEFTRAN into the SUNS shell provides a convenient software package for consequence assessments of individual scenarios.

Risk assessment in this context was carried out for a hypothetical bedded salt site (Cranwell, et al., 1987). The statistical sampling code used was Latin Hypercube Sampling (LHS) (Iman and Shortencarier, 1984) and the groundwater flow and radionuclide transport code used was NWFT/DVM (Campbell, et al., 1981). The Latin Hypercube and Monte Carlo sampling techniques and the rank correlation scheme of the LHS code are contained in the SUNS package. The NEFTRAN model used here is an enhanced version of NWFT/DVM. Thus, although the computing capability is similar to that used in Cranwell, et al. (1987), the mechanics of the problem solving can be accomplished much more conveniently using the SUNS/NEFTRAN package.

There are at least three reasons that the application is easier with SUNS. First, by operating on appropriate microcomputers, the SUNS/NEFTRAN package is transportable and interactive, with graphical and tabularized results immediately available. Several individuals can make test runs and participate in the early decisions to be made regarding the appropriateness of input data and model capabilities. Second, if it is found necessary to restart the analysis, the initial input can be easily modified using the editing capabilities of SUNS. Third, quality assurance is easier. It is usually necessary with batch or interactive commands to copy or rename input files, output files, and plot files when moving data from one software package to another. If this process is not totally automated, there is always the concern that a plot or output list may not be traceable back to an input file. The SUNS package provides quality assurance by handling files internally and by recording date and time of input file creation/modification and of execution. The latter appears on all SUNS-generated plots.

An example of a SUNS/NEFTRAN execution follows. There is no attempt to reproduce the analysis of Cranwell, et al.(1987), nor can the full capabilities of SUNS/NEFTRAN be demonstrated. One specialized application is run for a representative five member decay chain and a fictitious groundwater release scenario. The input file contains both fixed and variable data. All the output discussed below results from a single execution of the package.

The fixed data was run through NEFTRAN and an output data block containing time-dependent discharge rates was generated. Figure 5 is a hardcopy from the SUNS output processor showing discharge rates for the five isotopes from zero to 10^4 years. Other output options for time-dependent results include concentrations at the discharge point and drinking-water doses. Integrating the rate curves and dividing the integrated discharge for each isotope by some normalization (e.g., the EPA weighting factors), the results can be summed and compared to regulatory standards. This problem was based on EPA weighting factors for a radioactive waste repository containing 50,000 MTHM, of which 2 to 3 percent was accessed by circulating ground water. The total normalized discharge (0.55) is less than the regulatory limit (1.0) for the fixed data input.

The second part of the application assigns distributions on representing uncertainties to several input quantities including retardation factors for each isotope, fluid velocities, leach rate and dispersivity. All distributions were sampled using Latin Hypercube Sampling and NEFTRAN was executed for 100 repeated trials. Since a single input file was used, the second data block (containing weighted discharges) was appended to the first. Figure 6 shows a complementary cumulative distribution function (CCDF) drawn for the response variable called Weighted Discharge. As can be seen the regulatory limit is exceeded for about 10% of the trials. Using accepted definitions, the risk from this fictitious scenario can be calculated by multiplying the consequences predicted here by the probability of occurrence of the scenario. Thus, if the probability were near unity, risk would exceed standards for 10% of the trials.

Simple and partial correlation coefficients on ranks between weighted discharge and several input variables are shown in Table 1. These results indicate that retardation factors for plutonium, americium, and uranium, together with fluid velocity and leach rate make the greatest contributions to uncertainty in predicted values of weighted discharge. If this analysis had been performed for a real site, these correlation results could be useful in directing further data collection efforts.

IV. SUMMARY AND CONCLUSIONS

A microcomputer software package has been developed that considerably simplifies the application of Monte Carlo techniques in areas such as probabilistic safety assessment, risk assessment, and reliability analysis. The Sensitivity and Uncertainty Analysis Shell (SUNS) provides a menu-driven environment, an input editor, interactive graphics and statistics output, and complete file management capabilities. SUNS has been demonstrated by application to the release of radionuclides from a geologic disposal facility for radioactive waste.

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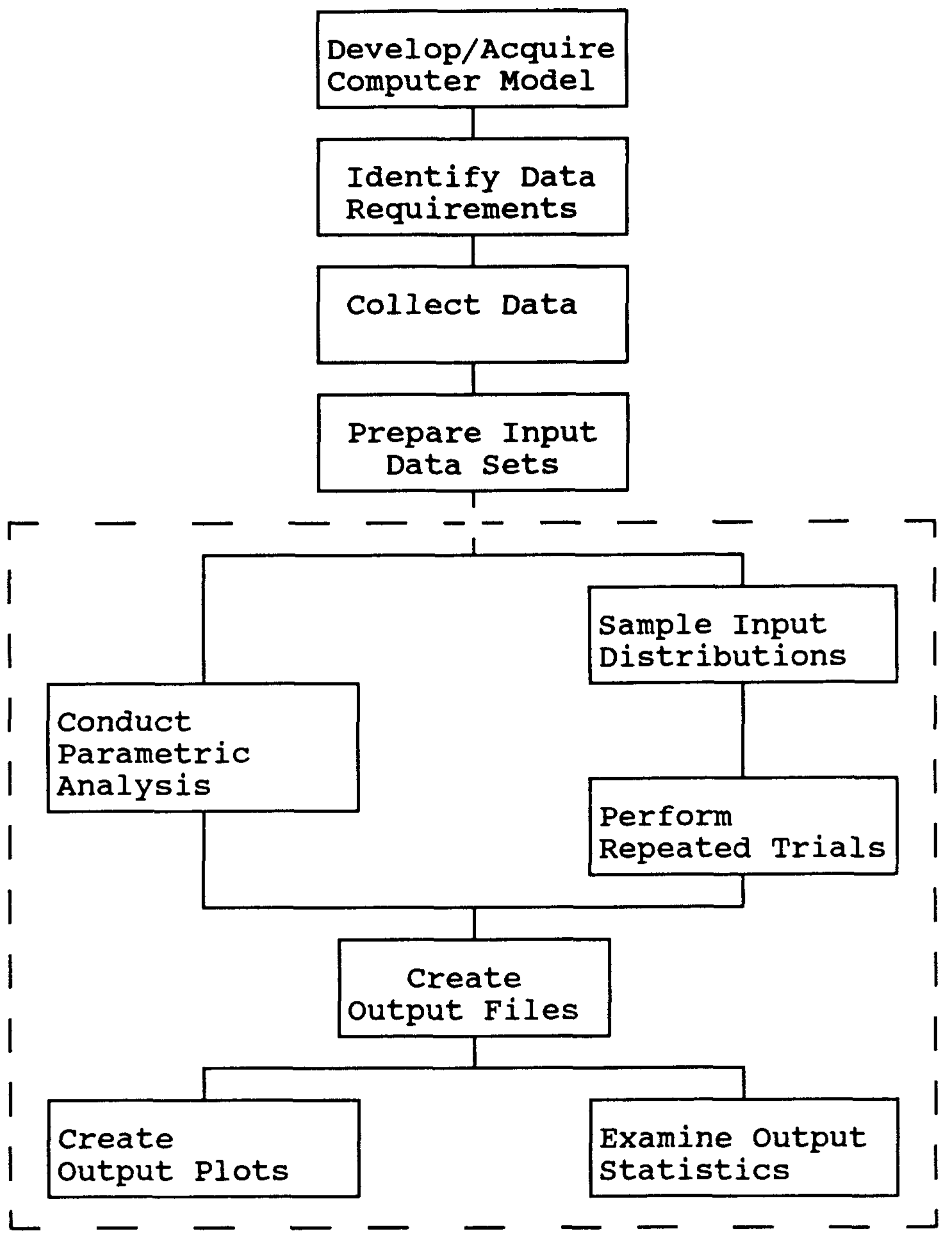


Figure 1. Structure of Typical Monte Carlo Analysis

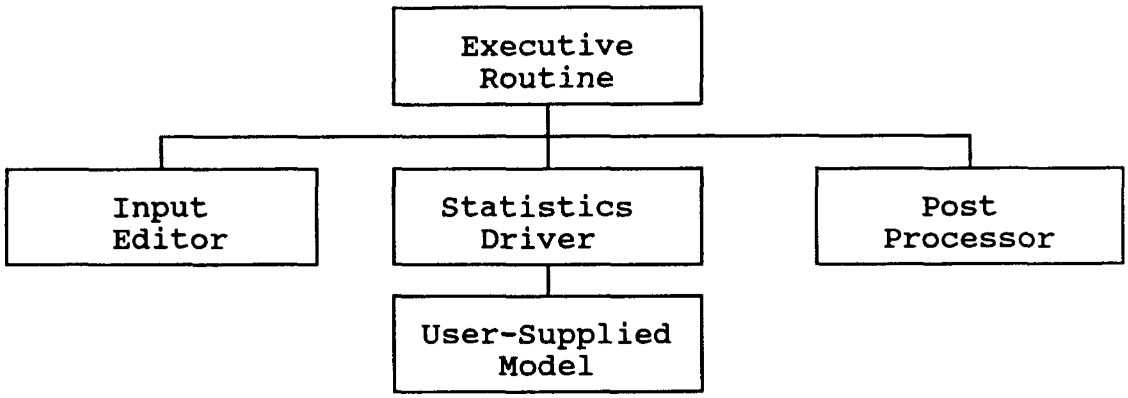


Figure 2. Structure of the SUNS Software Package

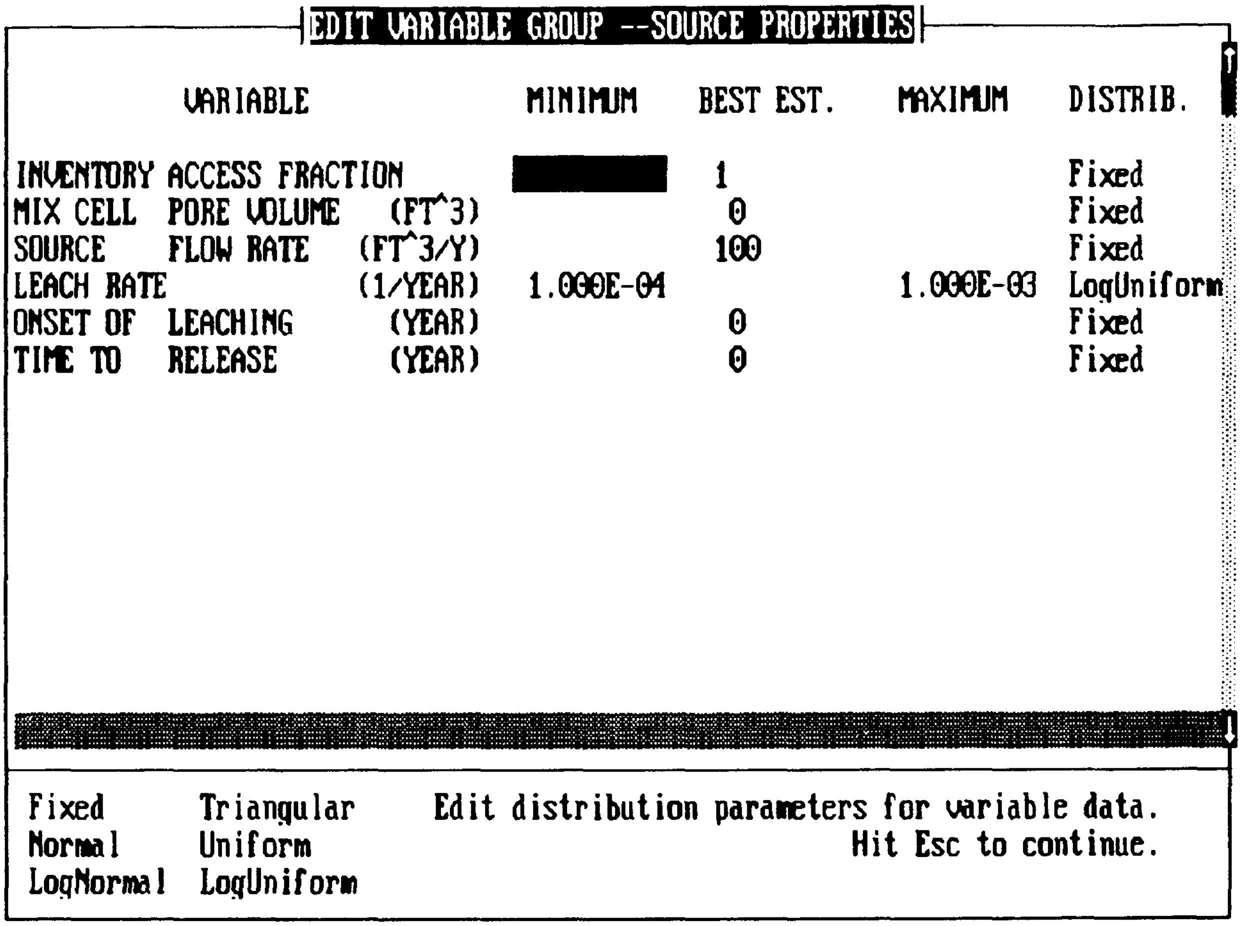


Figure 3. Example SUNS Input Screen
for Some Source Variables

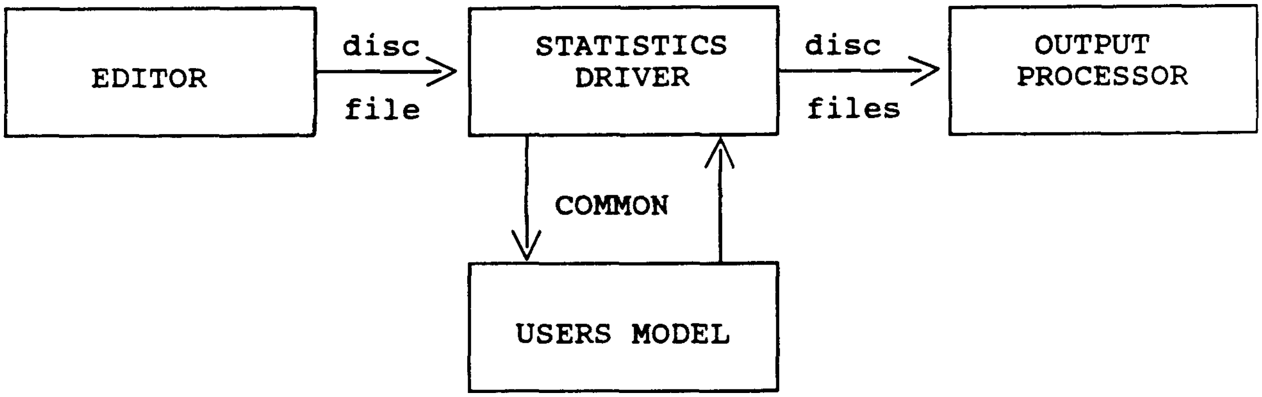
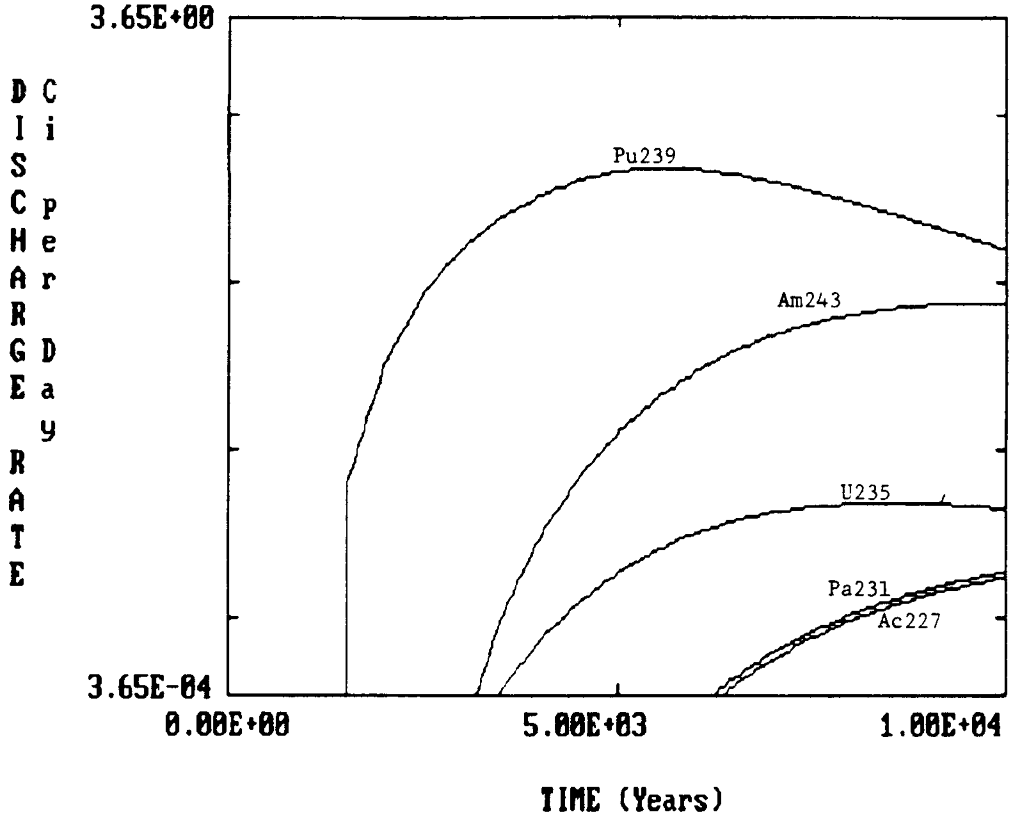


Figure 4. Information Transfer for the SUNS Package



EXAMPLE PROBLEM FOR POST-SMIRT SEMINAR

SMIRT.INP Created 11:29:47 on 05-22-1989. Run 11:29:59 on 05/22/1989.

Figure 5. Discharge Rates vs. Time for the 5-Member Decay Chain

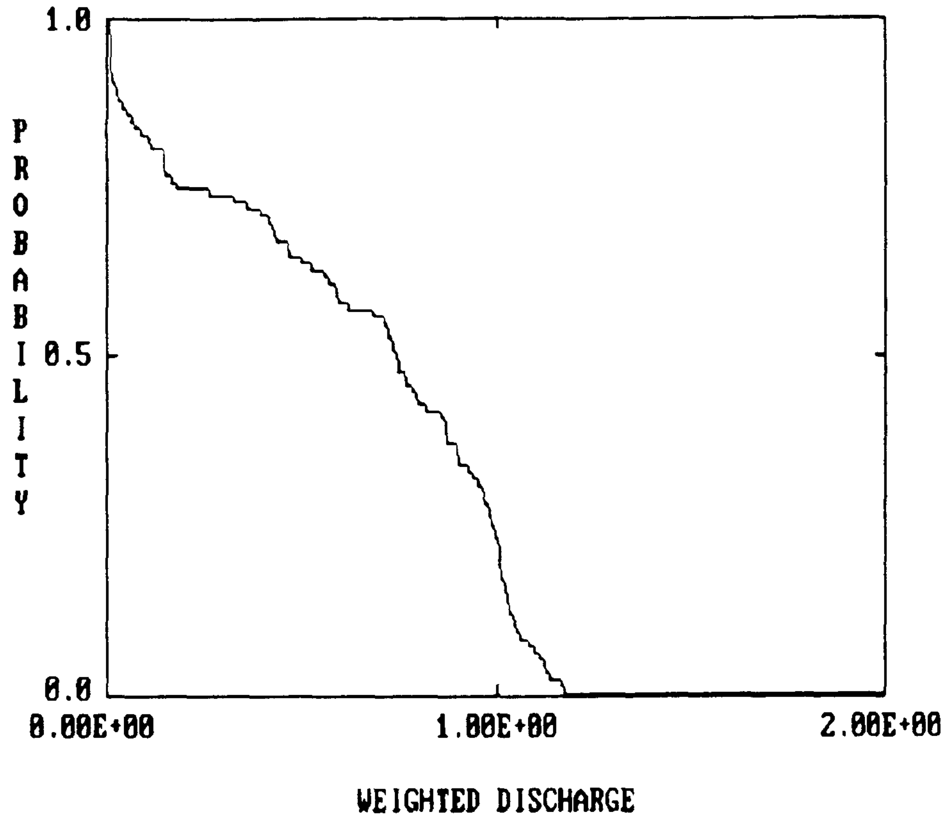


Figure 6. CCDF for Weighted Discharge

Table 1

Simple and Partial Correlation Coefficients on Ranks

VARIABLE	PARTIAL	SIMPLE
Plutonium Retardation	-0.64	-0.81
Fluid Velocity	0.62	0.43
Americium Retardation	-0.58	-0.80
Leach Rate	0.50	0.15
Uranium Retardation	-0.27	-0.75
Dispersity	0.12	0.05