Parameter Sensitivity Analyses of Modeling Results for the Yucca Mountain Repository from NRC's TPA 3.2 Computer Code

by

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September 1999

Summary and Conclusions

A statistical method was used with parameter sensitivity analyses to evaluate results from execution of the TPA Version 3.2 code. The TPA results consisted of several 500 realization sets of Monte Carlo runs pertaining to a base case scenario with a limited number of sampled parameters. Previously, several types of statistical and non-statistical techniques have been used to perform sensitivity analyses employing the TPA Version 3.2 code. The focus of this report was on a statistical test in which the 500 vectors for the 50,000-year time period of interest were sorted into two bins depending on whether the dose was greater or less than 0.2 mrem. The sampled parameters in each bin were then compared statistically to identify any statistical differences between the two bins. For the 50,000-year time period of interest, several parameters were found most influential for the analysis of this limited base case scenario study. The final list of influential parameters was selected on the basis of the K-S test, the Mann-Whitney U test, and the visual inspection of the cumulative probability curves.

Introduction

Yucca Mountain Project

Based on the provisions of the Nuclear Waste Policy Act (NWPA) and the Energy Policy Act (EnPA), the Nuclear Regulatory Commission (NRC) is responsible for evaluating the license application for a proposed geologic repository constructed for the emplacement of high-level nuclear waste at Yucca Mountain, Nevada. As groundwork for its regulatory review activities outlined in the NWPA and EnPA, the NRC is conducting detailed technical performance assessments to understand and identify the potentially important isolation characteristics and capabilities of the proposed repository system at the Yucca Mountain site based on the information currently available. An important facet of these performance assessment endeavors is the use of the Total -system Performance Assessment computer code.

Total-System Performance Assessment Code

The TPA code is designed to simulate the behavior of the geologic repository by taking into account the essential characteristics of the natural and engineered barrier systems, and the availability of information about the geologic setting and design. This document presents sensitivity analyses using the latest version of the TPA code, Version 3.2. One of the fundamental purposes for applying the TPA Version 3.2 code to the proposed repository is to acquire a detailed and quantitative understanding of the key factors controlling the degradation of the engineered barrier system, the release of the waste from the repository, the ensuing transport of the waste through various pathways, and possible human exposure at the location of the designated receptor group. A probabilistic method is used to model the total repository system that takes into account significant physical and chemical processes, as well as potentially disruptive events and processes.

This paper describes a particular sensitivity analysis technique utilized with results of the TPA Version 3.2 code system-level calculations. In general, a sensitive parameter is defined as one that provides a relatively large change in the output variable for a unit change in an input parameter. The goal of the sensitivity analyses presented in this report is to determine the parameters to which groundwater peak dose in the 50,000-year time period of interest shows the most sensitivity. The analyses were conducted for a basecase-type study using a limited number of sampled parameters without including any igneous activity or faulting disruptive events.

The technique used relies on the Monte Carlo method for probabilistic determining system performance. This sensitivity analysis of the system focuses on the groundwater peak dose in the 50,000-year time period of interest to an average member of a receptor group located 20-km from the repository. Many of the input parameters are not precisely known and are variable, so their values are described by probability distributions. The Monte Carlo technique makes repeated calculations called realizations of the possible states for the system, choosing values for the input parameters from their probability distributions. As many as 52 parameters are sampled in this analysis of the TPA Version 3.2 code, however only a few of these parameters contribute significantly to the uncertainty in peak doses because of the great sensitivity of peak doses to those parameters. It is assumed that the behavior of the system is simulated by appropriately sampling the random parameters and then computing the system

output for each realization. Since it is assumed that the decisions about appropriate model assumptions have been made in advance, no additional considerations are made concerning the dependence of the output on those assumptions.

Analyses Methods: Nonparametric Tests

Nonparametric tests, also sometimes referred to as distribution free tests, are often used in place of their parametric counterparts when certain assumptions about the underlying populations are questionable. All tests involving ranked data are nonparametric. This class of tests doesn't depend upon knowing the distribution of the results, nor upon knowing the mean value or knowing the standard deviation, so they can be applied more generally. Because of that fact, they are often more powerful in detecting population differences when certain assumptions are not satisfied. However, users of these tests must be aware that they are not necessarily as likely to detect significant effects, since they do not require quantitative dependent variables and do not require Gaussian distributions.

The analyses' methods presented in this paper consist of the following two nonparametric tests, which are described in detail below.

Mann-Whitney U Test

The Wilcoxon Mann-Whitney Test, also known as the Wilcoxon rank sum test, is one of the most effective of the nonparametric tests for comparing two populations. It is used to test the null hypothesis that two populations have identical distribution functions against the alternative hypothesis that the two distribution functions differ only with respect to location (median), if at all. The Wilcoxon Mann-Whitney test does not require the assumption that the differences between the two samples are normally distributed. In many applications, the Wilcoxon Mann-Whitney Test is used in place of the two-sample t-test when the normality assumption is questionable. This test can also be applied when the observations in a sample of data are ranks, that is, ordinal data rather than direct measurements.

To use the Mann-Whitney U test appropriately for statistical analyses, the following assumptions must be made:

- Within each sample, the values are independent, and identically distributed. The distribution does not need to be specified, but all the values in each sample follow the same continuous distribution.
- The two samples are independent of each other.
- The populations from which the two samples were taken differ only in location. That is, the populations may differ in their means or medians, but not in their dispersions or distributional shape (such as skewness).
- Because the test statistic for the Mann-Whitney rank sum is based only on the ranks within each sample, the test can be performed when the only data available are those relative ranks.

Kolmogorov-Smirnov Test (K-S Test)

For a single sample of data, the Kolmogorov-Smirnov nonparametric test is used to test whether or not the sample of data is consistent with a specified distribution function. When there are two samples of data, it is used to test whether or not these two samples may reasonably be assumed to come from the same distribution. The Kolmogorov-Smirnov test does not require the assumption that the population is normally distributed.

The K-S test is a goodness-of-fit test for any distribution. The test relies on the fact that the value of the sample cumulative density function is asymptotically normally distributed. To apply the K-S test, the cumulative frequency (normalized by the sample size) of the observations is calculated as a function of class, the cumulative frequency for a true distribution (most commonly, the normal distribution) is then calculated, and then the greatest discrepancy between the observed and expected cumulative frequencies, which is called the "D-Statistic", is determined. This value is compared against the critical D-statistic for that sample size. If the calculated D-statistic is greater than the critical one, then the null hypothesis that the distribution is of the expected form is rejected. Failure to understand and properly apply uniform distribution tests by the K-S test may result in drawing erroneous conclusions from your data.

Methods

Total-System Performance Assessment (TPA) Code: Data Input, Execution, & Output Files

The TPA Version 3.2 code is executed in batch mode using primary and some auxiliary input data files. Primary input data for the TPA Version 3.2 code are contained in the *tpa.inp* file. The *tpa.inp* file contains the information necessary for the user to specify the configurations, number of realizations, simulation time, number of subareas, and parameters to be sampled. The input data for the TPA Version 3.2 Code was prepared by modifying the *tpa.inp.meanvalues* file, which contains the mean values for all quantitative parameters contained in the TPA code. A limited number of parameters were selected and changed to their values as listed in *tpa.inp.basecase*. Once the alterations to the *tpa.inp* file were completed, the TPA Version 3.2 code was executed in a UNIX operating system with the command *tpa.e*.

During execution, the TPA Version 3.2 code generated a number of output files. Four of these files were used in the sensitivity analyses described in this paper. The output files of interest to this project are as follows:

Output Files Used for Calculation Purposes

(1) *gwpkdos.res* – data file containing the total groundwater peak dose, time of peak dose, and dose from each nuclide at the time of peak dose.

(2) *samplpar.res* – data file consisting of the sample parameter values for each vector

Output Files Used for Labeling and Identification Purposes

(3) *samplpar.abb* – header file for samplpar.res with sampled parameter abbreviations

(4) *samplpar.hrd* – header description file for samplpar.res with sampled parameter abbreviations accompanying the complete sampled parameter names.

The TPA Version 3.2 code was executed for three separate 500-realization runs, which are as follows:

(1) Run 1 consisted of an input file with mean values for all parameters except for 52 parameters selected to be sampled. There were no parameter correlations introduced in this run. Also, the input file provided a seven-subarea discretization of the repository.

(2) Run 2 consisted of an input file with mean values for all parameters except for 52 parameters selected to be sampled. Parameter correlations were introduced for pairs represented within the 52 sampled parameters. Also, the input file provided a seven subarea discretization of the repository.

(3) Run 3 consisted of an input file with mean values for all parameters except for 40 parameters selected to be sampled. Parameter correlations were introduced for pairs represented within the 52 sampled parameters. Also, the input file was modified to define the repository area as one rectangular subarea to minimize the number of loops required for each realization during the execution of the TPA Version 3.2 code.

Dose Criteria

To simulate a regulatory approach, a dose criterion for the total groundwater peak dose (as contained in the *gwpkdos.res* file) at the 50,000-year time period of interest was initially chosen as 1.0 millirem. This criterion was only utilized with the results for Run 1. The output files of all the runs were processed using a total groundwater peak dose criterion of 0.2 mrem.

Code to Bin Acceptable/Unacceptable Realizations Based on the Chosen Dose Criteria

A FORTRAN computer code was written (see Appendix A) that processes the data contained in the *gwpkdos.res* file by determining whether the total groundwater peak dose at the 50,000-year time period of interest is greater than, equal to, or less than the selected dose criterion. Realizations resulting in peak doses less than the dose criterion were denoted as behaviors and realizations resulting in peak doses greater than or equal to the dose criterion were denoted as non-behaviors. This computer code also writes the values of the sampled parameters for behaviors in one file (*behaviorfile*) and for non-behaviors in a second file (*nonbehavefile*).

General Sensitivity (GENSEN) Program

The GENSEN program is a FORTRAN program created by G.M. Hornberger and R.C. Spear (see Appendix B for additional details) which analyzes the differences between the two bins of parameters from the *behaviorfile* and *nonbehavefile* by looking at covariances as well as simple univariate separations. This statistical investigation is accomplished by using the Kolmogorov-Smirnov and the Mann-Whitney U tests as described above.

The Kolmogorov-Smirnov statistic (denoted as DAA in the GENSEN program) is the difference between cumulative distribution function curves. The critical statistic is the maximum distance between the two cumulative curves. The critical value of the difference was chosen at the 95-percent confidence level; when the difference was greater than that, the two curves were considered statistically different. The parameters from both behavioral and non-behavioral situations were mapped onto a standardized probability axis for plotting. In the GENSEN

program, this value is denoted as "U" (the Mann-Whitney statistic). The underlying cumulative probability associated with the parameter is labeled "PROB". The other values listed in the output tables from GENSEN are SNB-the cumulative probability under behavior, SNNB-the cumulative probability under non-behavior, DELB-distance between underlying and behavior, DELNB-distance between underlying and non-behavior, and DELBNB-distance between behavior and non-behavior.

Analysis of Output from the GENSEN Program

The output from the GENSEN program was analyzed in two interdependent ways. (i) The DAA values for each parameter were used to rank order them; this yielded a straightforward sensitivity ranking for all the sampled parameters. (ii) Cumulative probability plots were constructed by plotting U (the Mann-Whitney statistic) against SNB and SNNB (the cumulative probabilities under behavior and non-behavior, respectively). The cumulative probability plots were visually inspected to determine which parameters displayed the biggest differences, which correlates to large DAA values and to ensure that the K-S test did not yield any false results. This analysis was completed with the results of four different configurations. These configurations and their distinguishing characteristics are listed in Table 1.

Table 1: Description of Configurations Used in this Sensitivity Analysis

Configuration	1	2	3	4
Data from Run #	1	1	2	3
# of Parameters	52	52	52	40
# of Realizations	500	500	500	500
Correlated Input Parameters?	No	No	Yes	Yes
Dose Criteria (mrem)	1.0	0.2	0.2	0.2
# of Subareas	7	7	7	1

Results

Parameter Ranking by DAA Statistic

For each of the four configurations considered, the top ten parameters as assessed by the ranking of their DAA values yielded from the GENSEN program are listed in Table 2. Please refer to Appendix C for a complete listing of all the sampled parameters, their DAA values, and their rankings for each of the four configurations.

Table 2: Top Ten Parameters Based on the Ranking of DAA Values for Four Configurations

Ranking	Configuration 1	Configuration 2	Configuration 3	Configuration 4
1	ARDSAVNp	SbArWt%	SbArWt%	SFWt%C1
2	MAPM@GM	WPRRG@20	AAMAI@S	SbArWt%
3	APrs_SAV	MAPM@GM	WPRRG@20	AAMAI@S
4	RD_IV_I	APrs_SAV	MAPM@GM	MAPM@GM
5	ARDSAV_I	ARDSAV_I	APrs_SAV	APrs_SAV
6	WPRRG@20	ARDSAVNp	Fow*	WPRRG@20
7	RD_IV_Ra	SFWt%C5	ARDSAVPu	ARDSAV_I
8	MixZnT20	SFWt%C2	ARDSAVAm	Fow*
9	MATI@GM	RD_IV_I	ARDSAVNp	MixZnT20
10	ARDSAVRa	RD_IV_Np	ARDSAV_I	ARDSAVPu

Visual Inspection of Cumulative Probability Plots

As previously described, the cumulative probability plots for each of the top ten parameters for each analyzed configuration were constructed by plotting the Mann-Whitney statistic (U) against the cumulative probabilities under behavior and non-behavior (SNB and SNNB, respectively). Please refer to Appendix D for a full listing of these plots. Since the K-S test yields erroneous results under certain circumstances (see Figure 1 below), each cumulative probability plot for each of the statistically significant parameters was checked for this phenomenon. The results of this visual analysis are contained in Tables 3, 4, 5, and 6 below.

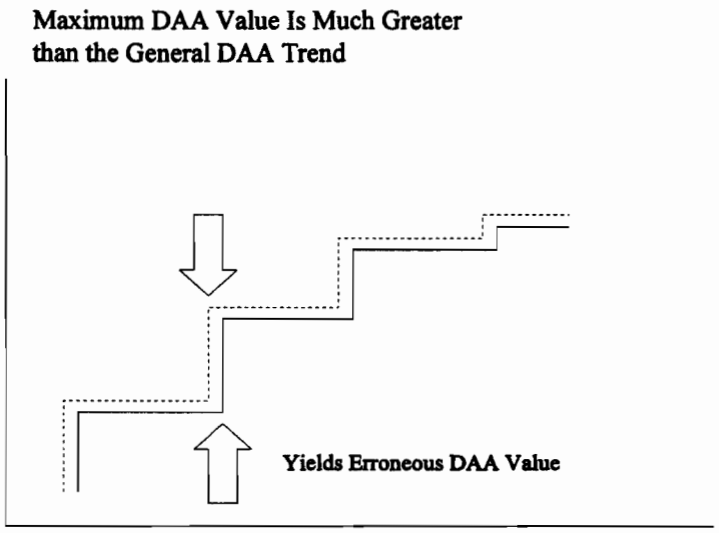


Figure 1: Example of K-S Test Yielding Erroneous Results, which Stresses the Importance of Visually Inspecting the Cumulative Probability Plots for Each Parameter

Table 3: Results For The Visual Inspection of the K-S Test Results for Configuration 1

Ranking	Parameter Name	Passed Visual Inspection (Yes or Questionable)
1	ARDSAVNp	Questionable
2	MAPM@GM	Yes
3	APrs_SAV	Questionable
4	RD_IV_I	Yes
5	ARDSAV_I	Yes
6	WPRRG@10	Questionable
7	WPRRG@20	Yes
8	RD_IV_Ra	Yes
9	MixZnT20	Questionable
10	MATI@GM	Yes

Table 4: Results For The Visual Inspection of the K-S Test Results for Configuration 2

Ranking	Parameter Name	Passed Visual Inspection (Yes or Questionable)
1	SbArWt%	Yes
2	WPRRG@20	Yes
3	MAPM@GM	Questionable
4	APrs_SAV	Questionable
5	ARDSAV_I	Yes
6	ARDSAVNp	Yes
7	SFWt%C5	Yes
8	SFWt%C2	Yes
9	RD_IV_I	Questionable
10	WPRRG@10	Questionable

Table 5: Results For The Visual Inspection of the K-S Test Results for Configuration 3

Ranking	Parameter Name	Passed Visual Inspection (Yes or Questionable)
1	SbArWt%	Yes
2	AAMAI@S	Yes
3	WPRRG@20	Yes
4	MAPM@GM	Questionable
5	APrs_SAV	Questionable
6	Fow*	Yes
7	ARDSAVPu	Yes
8	ARDSAVAm	Questionable
9	ARDSAVNp	Yes
10	ARDSAV_I	Yes

Table 6: Results For The Visual Inspection of the K-S Test Results for Configuration 4

Ranking	Parameter Name	Passed Visual Inspection (Yes or Questionable)
1	SFWt%C1	Yes
2	SbArWt%	Yes
3	AAMAI@S	Yes
4	MAPM@GM	Questionable
5	APrs_SAV	Questionable
6	WPRRG@20	Yes
7	ARDSAV_I	Yes
8	Fow*	Yes
9	MixZnT20	Questionable
10	ARDSAVPu	Yes

Parameters Found Significant in Both Analysis Methods

This portion of the paper presents the overall sensitivity analyses based on the statistical analysis of a 500-vector Monte Carlo analysis of a configuration involving a limited number of selected parameters to be sampled for the 50,000-year time period of interest. Table 7 contains the parameters that were determined to be significant for each configuration, which were determined as parameters that passed both the K-S test and the visual inspection of their cumulative probability plots.

Table 7: Influential Parameters that Have Satisfied the Sensitivity Requirements for the K-S Test and the Visual Inspection of their Cumulative Probability Profiles

Configuration	1	2	3	4
Influential Parameters	MAPM@GM	SbArWt%	SbArWt%	SFWt%C1
	RD_IV_I	WPRRG@20	AAMAI@S	SbArWt%
	ARDSAV_I	ARDSAV_I	WPRRG@20	AAMAI@S
	WPRRG@20	ARDSAVNp	Fow*	WPRRG@20
	RD_IV_Ra	SFWt%C5	ARDSAVPu	ARDSAV_I
	MATI@GM	SFWt%C2	ARDSAVNp	Fow*
	--	--	ARDSAV_I	ARDSAVPu

Discussion

Selection of Overall Influential Parameters

This portion of the paper attempts to identify influential parameters using the analyses presented above. For the 50,000-year time period of interest, several parameters were found most influential for the four configurations using a limited basecase scenario. Previously, a sensitivity analysis method consisting of a combination of the K-S test, the Mann-Whitney U test, and visual inspection of the cumulative probability curves was utilized to determine the most influential parameters. Since it is not clear that any one method is superior to another for this determination of sensitivity, the final list of parameters was selected on the combination of all the analytical methods used.

The selected parameters are presented in Table 8, which summarizes the sensitive parameters as determined by using an analysis method composed of a combination of the tests as described above for each statistically significant parameter. The scores listed in Table 8 specifies the number of configurations that selected a particular parameter among the ten most statistically significant. The parameters that did not make the final list include those that did not have statistically significant DAA values yielded by the K-S test and those that did not pass the visual inspection of the cumulative probability plot. It should be noted that there is one sampled parameter (the water use parameter at 10 km - WPRRG@10) which has been disregarded, because it is not used in the execution of the TPA code and therefore could not have had an effect on the results. The analyses resulted in only eight parameters being selected as influential for the 50,000-year time period of interest. It is apparent that significant variations can exist for this particular time period of interest.

Table 8: Overall Influential Parameters Determined for the 50,000-year Time Period of Interest from Sensitivity Analysis Studies

Parameter Abbreviation	Parameter Name	Score
SbArWt%	Subarea Wet Fraction	3/3
WPRRG@20	Well Pumping Rate at 20-km Receptor Group	3/3
ARDSAV_I	Alluvium R_d for ^{129}I	3/3
ARDSAVNp	Alluvium R_d for ^{237}Np	2/3
SFWt%C	Spent Fuel Wet Fraction for Corrosion Failures	2/3
AAMAI@S	Areal Average Mean Annual Infiltration at Start	2/3
Fow*	Flow focusing factor	2/3
ARDSAVPu	Alluvium R_d for ^{239}Pu	2/3

**** Note: The results of the statistical analyses for Configuration 1 were not used in the designation of overall influential parameters due to the selection of a different dose criterion (0.2 mrem) for the remaining configurations.**

Key Integrated Subissues for 50,000-year Time Period of Interest

Parameters that have been identified as influential for the 50,000-year time period of interest will be considered in conjunction with their corresponding NRC integrated subissues. These important connections are presented in Table 9.

Table 9: Influential Parameters for the 50,000-year Time Period of Interest with their Corresponding Integrated Subissues.

Integrated Subissues	Influential Parameters
Waste Package Degradation	Spent Fuel Wetted Fraction for Corrosion Event (SFWt%C)
Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms	Subarea Wet Fraction (SbArWt%) Flow Focusing Factor (Fow*)
Spatial and Temporal Distributions of Flow	Areal Average Mean Annual Infiltration at Start (AAMAI@S)
Retardation of Water Production Zones and Alluvium	Alluvium Matrix R_d for ^{129}I (ARDSAV_I) Alluvium Matrix R_d for ^{237}Np (ARDSAVNp) Alluvium Matrix R_d for ^{239}Pu (ARDSAVPu)
Dilution of Radionuclides in Groundwater through Well Pumping	Well Pumping Rate at Receptor Group at 20 km (WPRRG@20)

Discussion of Correlation Effects on Influential Parameters and Peak Dose

The effects of parameters in the models for the TPA code are due in large part to the deliberate correlations of several of the radionuclide retardation parameters, particularly those for neptunium, iodine, plutonium, and uranium. It is likely that some of these factors show up because of the large contribution to peak dose of ^{237}Np. In the case of ^{214}Am, some dose also may be indirectly attributed to ^{241}Am decaying to ^{237}Np.

The consequences of these correlated pairs can be ascertained by comparing the results of Run 2 with its non-correlated parameters and the results of Runs 3 and 4 (see Table 2), which were modified to include parameter correlations. Table 10 presents the correlations that were utilized in Runs 3 and 4.

Table 10: Correlations Between Two Input Parameters Selected to Be Utilized in the Execution of the TPA Version 3.2 Code.

Parameter 1 Correlated with Parameter 2		Correlation Factor
SbArWt%	AAMAI@S	0.631
Fow*	AAMAI@S	-0.224
Fow*	SbArWt%	-0.366
ARDSAVAm	ARDSAVPu	0.964
ARDSAVAm	ARDSAV_U	0.346
ARDSAVAm	ARDSAVNp	0.837
ARDSAVPu	ARDSAV_U	0.489
ARDSAVPu	ARDSAVNp	0.881
ARDSAVNp	ARDSAV_U	0.610

Before correlations were introduced, the subarea wet fraction and the alluvium matrix retardation values for iodine and neptunium were determined to be statistically significant and influential parameters. As a consequence of their correlations to other sampled parameters as introduced into Runs 3 and 4, three factors experienced large increases in their statistical significance. (1) The mean areal average infiltration into the subsurface at the start was ranked 42nd out of 52 parameters in Run 1, however when its positive correlation to the subarea wet fraction was added, it quickly transitioned from its initial stage as an unimportant parameter to one which ranked extremely high in the sensitivity analyses. (2) Another example of an extensive change stemming from the addition of a correlation is the alluvium matrix retardation value for americium; it was converted from 37th place in the Run 1 (with no correlations) to a significant position in the sensitivity results for Run 3, which contained a positive correlations for the alluvium matrix retardation values for americium and the retardation factors for plutonium and neptunium. (3) Once the alluvium matrix retardation value for uranium had been modified to include positive correlations between it and the retardation values for plutonium and neptunium, its parameter ranking value changed from 43rd to the 15th and 8th places in Runs 3 and 4, respectively.

Comparison to the Previous Sensitivity Analyses Using TPA Version 3.2 Code

Extensive sensitivity analyses using various statistical and non-statistical methods have been conducted with data resulting from the execution of TPA Version 3.2 Code. The influential

parameters for the 50,000-year time period of interest from sensitivity analysis studies are presented in Table 11.

Table 11: Influential Parameters for the 50,000-year Time Period of Interest from Sensitivity Analysis Studies

Parameter Abbreviation	Parameter Name
SbArWt%	Subarea Wet Fraction
WPRRG@20	Well Pumping Rate at 20-km Receptor Group
ARDSAVNp	Alluvium R_d for ^{237}Np
ARDSAVTc	Alluvium R_d for ^{99}Tc
Fmult*	Fmult factor for Water Flow Entering a Waste Package
ARDSAV_I	Alluvium R_d for ^{129}I
ARDSAV_U	Alluvium R_d for ^{234}U
AAMAI@S	Areal Average Mean Annual Infiltration at Start

A comparison was conducted between the results of the statistical analysis presented in this report and the results previously obtained from the statistical and non-statistical analysis of the investigation of a basecase scenario executed using the TPA Version 3.2 Code. Dependence of several parameters, particularly the flow focusing factor, the spent fuel wet fraction for corrosion failures, and the alluvium matrix retardation factor for ^{239}Pu, are suspicious, since these parameters were sampled but have not reliably shown up as significant in other sensitivity studies using TPA Version 3.2 code. Contradiction between the present analysis and previous analyses also occurs with the enigmatic absence of parameters previously deemed influential, such as the retardation factor for technetium and the Fmult factor.

Conclusions

The information yielded from execution of the TPA Version 3.2 code was used with sensitivity analyses to apply a statistical method to a 500 realization set of Monte Carlo runs pertaining to a basecase scenario with a limited number of sampled parameters. Even though several types of statistical and non-statistical techniques have been used to perform sensitivity analyses employing the TPA Version 3.2 code, the focus of this report was on a statistical test in which the 500 vectors for the 50,000-year time period of interest were sorted into two bins depending on whether the dose was greater or less than 0.2 mrem. The sampled parameters in each bin were then compared statistically to identify any statistical differences between the two bins.

For the 50,000-year time period of interest, several parameters were found most influential for the analysis of this limited basecase scenario study. The final list of influential parameters (see Table 8) was selected on the combination of all the K-S test, the Mann-Whitney U test, and the visual inspection of the cumulative probability curves. The most influential parameters were determined as follows:

- Subarea Wet Fraction
- Well Pumping Rate at 20-km Receptor Group
- Alluvium Rd for 129I

This study resulted in determining three influential parameters (the mean areal average infiltration into the subsurface at the start, the subarea wet fraction, the flow focusing factor, and the spent fuel wet fraction for corrosion failures) whose primary effects were altering the spatial and temporal distributions of flow, the quantity and chemistry of the flow of water, the contacting of water with the waste packages, and the subsequent waste package degradation and eventual failure. Insight provided also by this study included highlighting the importance of alluvium matrix retardation factors for various radionuclides including ^{237}Np, ^{129}I, and ^{239}Pu. As supported by previous scientific evidence and sensitivity studies as well as this report, the retardation factor for ^{237}Np is of upmost importance because the large peak doses for any radionuclide for any type of realization comes from ^{237}Np. Since the retardation of radionuclides in the alluvium matrix has been determined as been identified as influential parameters, it follows that the dilution of radionuclides in groundwater through well pumping is also a parameter that is essential to the peak dose.

The investigation of integrated subissues along with their corresponding influential parameters suggests that the geologic repository for the containment of high-level nuclear waste in Yucca Mountain may provide better total-system performance with the introduction of additional engineered characteristics. The results of this report focuses on the necessity to provide better methods for controlling the flow of water onto and eventually into failed waste packages, as well as to constrain radionuclide sorption in the alluvium that to help cause a significant decrease in radionuclide transport or a longer delay in the arrival time of radionuclides at the location of the selected receptor group.

REFERENCES

Probability and Statistics for Engineers second edition
Irwin Miller
John E. Freund
Prentice-Hall, Inc.
Englewood Cliffs, New Jersey 07632
1977

Probabilistic Modeling and Analysis in Science and Engineering
T.T. Soong
John Wiley & Sons Inc
New York
1981

Bayesian Reliability Analysis
Harry F. Martz
Ray A. Waller
Krieger Publishing Company
Malabar, Florida
1982

Draft of Total-System Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and User's Guide
Prepared for Nuclear Regulatory Commission Cotnract NRC-02-97-009
Prepared by the Center for Nuclear Waste Regulatory Analyses
September 1998

System-Level Repository Sensitivity Analyses Using TPA Version 3.2 Code
Prepared for Nuclear Regulatory Commission Contract NRC-02-97-009
Prepared by the Center
August 1999

APPENDIX A

NAMES OF SAMPLED PARAMETERS (NON-CONSTANT)		
arameter ID #	Abbreviation	Full Name
1	AAMAI@S	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
2	MAPM@GM	MeanAveragePrecipitationMultiplierAtGlacialMaximum
3	MATI@GM	MeanAverageTemperatureIncreaseAtGlacialMaximum[degC]
4	FOC-R	FractionOfCondensateRemoved[1/yr]
5	FOCTR	FractionOfCondensateTowardRepository[1/yr]
6	FOCTR-R	FractionOfCondensateTowardRepositoryRemoved[1/yr]
7	AA_2_1	AA_2_1[C/m2/yr]
8	*Chlorid	ChlorideMultFactor
9	Fow*	FowFactor
10	Fmult*	FmultFactor
11	SbArWt%	SubAreaWetFraction
12	WP-Def%	DefectiveFractionOfWPs/cell
13	RD_IV_Pu	RD_Invert_Pu
14	RD_IV_U	RD_Invert_U
15	RD_IV_Am	RD_Invert_Am
16	RD_IV_Np	RD_Invert_Np
17	RD_IV_Th	RD_Invert_Th
18	RD_IV_Ra	RD_Invert_Ra
19	RD_IV_Pb	RD_Invert_Pb
20	RD_IV_I	RD_Invert_I
21	RD_IV_Tc	RD_Invert_Tc
22	RD_IV_Ni	RD_Invert_Ni
23	RD_IV_Se	RD_Invert_Se
24	RD_IV_Nb	RD_Invert_Nb
25	SFWt%I1	SFWettedFraction_Initial_1
26	SFWt%I2	SFWettedFraction_Initial_2
27	SFWt%I3	SFWettedFraction_Initial_3
28	SFWt%I4	SFWettedFraction_Initial_4
29	SFWt%I5	SFWettedFraction_Initial_5
30	SFWt%I6	SFWettedFraction_Initial_6
31	SFWt%I7	SFWettedFraction_Initial_7
32	SFWt%C1	SFWettedFraction_Corrosion_1
33	SFWt%C2	SFWettedFraction_Corrosion_2
34	SFWt%C3	SFWettedFraction_Corrosion_3
35	SFWt%C4	SFWettedFraction_Corrosion_4
36	SFWt%C5	SFWettedFraction_Corrosion_5
37	SFWt%C6	SFWettedFraction_Corrosion_6
38	SFWt%C7	SFWettedFraction_Corrosion_7
39	InvMPerm	InvertMatrixPermeability[m^2]
40	ARDSAVAm	AlluviumMatrixRD_SAV_Am
41	ARDSAVNp	AlluviumMatrixRD_SAV_Np
42	ARDSAV_I	AlluviumMatrixRD_SAV_I
43	ARDSAVTc	AlluviumMatrixRD_SAV_Tc
44	ARDSAV_U	AlluviumMatrixRD_SAV_U
45	ARDSAVPu	AlluviumMatrixRD_SAV_Pu
46	ARDSAVRa	AlluviumMatrixRD_SAV_Ra
47	ARDSAVSe	AlluviumMatrixRD_SAV_Se
48	APrs_SAV	AlluviumMatrixPorosity_SAV
49	WPRRG@20	WellPumpingRateAtReceptorGroup20km[gal/day]
50	PlumeTh5	PlumeThickness5km[m]
51	AqThick5	AquiferThickness5km[m]
52	MixZnT20	MixingZoneThickness20km[m]

APPENDIX B

APPENDIX B

BEHAVELINK.F:
A CODE TO BIN REALIZATIONS BASED ON A CHOSEN DOSE CRITERION

Behavelink.f is a FORTRAN computer code that was written to process the data contained in the *gwpkdos.res* file (an output file created by the execution of TPA Version 3.2 code) by determining whether the total groundwater peak dose at the 50,000-year time period of interest is greater than, equal to, or less than the selected dose criterion. Realizations resulting in peak doses less than the dose criterion were denoted as behaviors and realizations resulting in peak doses greater than or equal to the dose criterion were denoted as non-behaviors. This computer code also writes the values of the sampled parameters for behaviors in one file (*behaviorfile*) and for non-behaviors in a second file (*nonbehavefile*). The code is also versatile; it is equipped to easily handle modifications by the user, including changes to the value for the chosen dose criterion, the number of sampled parameters, the number of realizations, as well as the names for the output files.

```
      Program BehaveLink
C
C       Declarations
C       array v initialized with number of realizations and parameters
        real*4 v(500,52)
C
C       pkdose.inp is input file containing numbers of vectors
        open (unit=5, file='pkdose.inp')
C
C       skip first four lines of input file (heading)
        do i=1,4
          read (5,*)
        end do
C
C       Initial arrays to zero
        open (11,file='gwpkdos.res')
        open (12,file='samplpar.res')
        open (13,file='samplpar.abb')
        open (21,file='behaviorfile')
        open (22,file='nonbehavefile')
C
C       read number of vectors
        read (5,*) nvector
C       skip first 8 lines of input file 8 (header lines)
        do i=1,8
          read(11,*)
        end do
C       skip first 7 lines of input file 12 (header lines)
        do i=1,7
          read(12,*)
        end do
C       skip first 5 lines of input file 13 (header lines)
        do i=1,5
          read(13,*)
        end do
C
C       Labeling output files
        write (21,*)
        write (22,*)
        write (21,*) 'Behavior File'
        write (22,*) 'Non-Behavior File'
        do i=1,5
        write (21,*)
        write (22,*)
        end do
```

Program BehaveLink (cont'd)

```
C       write parameter numbers
        do vl=1,52
        write (21,*) vl
        write (22,*) vl
        end do
C       binning using dose criteria
        do nv=1, nvector
          read (11,*) vector, pktime, pktede
           If (pktede.LT.(2e-4)) then
             read (12,*) vectorn
             read (12,*)(v(i,j),j=1,52)
             write (21,'(12x,15e7.1e2)')(v(i,j),j=1,52)
           else
        read (12,*) vectorn
        read (12,*)(v(i,j),j=1,52)
        write (22,'(12x,15e7.1e2)')(v(i,j),j=1,52)
          endif
        end do
        end
```

APPENDIX C

GENSEN.F:
A GENERAL SENSITIVITY PROGRAM FOR STATISTICAL ANALYSES

GENSEN.f is a FORTRAN program created by G.M. Hornberger and R.C. Spear (see Appendix B for additional details) which analyzes the differences between the two bins of parameters from two input files (*behaviorfile* and *nonbehavefile*) by looking at covariances as well as simple univariate separations. This statistical investigation is accomplished by using two nonparametric tests: the Kolmogorov-Smirnov and the Mann-Whitney U tests. This code is also adjustable; it is can be quickly modified to process input files with any given number of parameters. The example given in this appendix has been altered to compensate for statistical calculations involving 52 sampled parameters.

```
      PROGRAM GENSEN
C
C     STATISTICS FOR GENERALIZED SENSITIVITY ANALYSIS
C      KOMOGOROV-SMIRNOV STATISTIC; FUKUNAGA-KOONTZ TRANSFORMATION
C
C     PROGRAM BY G.M.HORNBERGER AND R.C.SPEAR APRIL 1978(CANBERRA)
C                          REVISED AUG (GMH) 1979(BERKELEY)
C                          REVISED (BJC) 1983(CVILLE)
c                          adapted for pc (gmh) 1986(cville)
c                           {LAHEY FORTRAN}
c                          further modified and commented for
c                           pc  bjc (1987) cville
C
C     FOR INFORMATION CONTACT G.M.HORNBERGER
C                     DEPT. ENVIRON. SCI.
C                     CLARK HALL
C                     UNIVERSITY OF VIRVINIA
C                     CHARLOTTESVILLE, VA 22903
C     ************************************************************
C
C     SELECTED VARIABLE LIST:
C          PSI-PARAMETER VECTOR
C          NB -BEHAVIOR CODE
C          LAB-PARAMETER LABEL
C          NPAR-NUMBER OF PARAMETERS
C          N5 -NUMBER OF REPLICATIONS
C          VMAP -MAPPED PARAMETER VECTOR
C          MAP-CODE FOR EXECUTION:
C              =0 FOR STATISTICS IN ORIGINAL PARAMETER SPACE
C              =1 FOR F-K TRANSFORMATION BEHAVIORS
C              =2 FOR F-K TRANSFORMATION NON-BEHAVIORS
C              =3 FOR ALL THREE ABOVE
C              =4 FOR ORIGINAL AND BEHAVIOR ONLY
C     ************************************************************
C
C     DECLARATIONS:
C
       CHARACTER*10 TITLE(7),LAB(52),LIN(100),CBL,CBB,CNN,LB1(52),
     2          LB2(52)
      CHARACTER*20 fileb,filenb,fileout,lbb*10,lbnb*10
       LOGICAL*4 LFLAG
      DIMENSION PSI(3000,52),NB(3000),VMAP(3000,52),COVB(52,52),
     2 COVNB(52,52),XMB(52),XMNB(52),EV(52,52),EVAL(52),
     3 AA(52,52),BB(52,52),DD(52,52),A(3000),B(3000),
     4 CC(52,52),C1(52,52),C2(52,52),UG(19),
     5 SNN1(50),SNN2(50),XMBNB(52),EVALB(52),D1(6),D2(6),
     6 XMEAN(52),VAR(52),COVBNB(52,52),CT(52,52),EVB(52,52)
```

Program GENSEN (cont'd)

```
      DATA UG/-1.643,-1.285,-1.037,-.845,-.676,-.528,
     2  -.386,-.255,-.128,0.,.128,.255,.386,.528,.676,
     3  .845,1.037,1.285,1.643/
      DATA D2/1.22,1.36,1.48,1.63,1.73,1.95/
      DATA CBL/'         '/
      DATA CBB/'BBBBBBBBBB'/
      DATA CNN/'NNNNNNNNNN'/
      DATA LBB/'BEHAVIOR= '/
      DATA LBNB/'NOTBEHAV= '/
     DATA LB1/'EVB(1)   ','EVB(2)   ','EVB(3)   ','EVB(4)   ',
     2       'EVB(5)   ','EVB(6)   ','EVB(7)   ','EVB(8)   ',
     3       'EVB(9)   ','EVB(10)  ','EVB(11)  ','EVB(12)  ',
     4       'EVB(13)  ','EVB(14)  ','EVB(15)  ','EVB(16)  ',
     5       'EVB(17)  ','EVB(18)  ','EVB(19)  ','EVB(20)  ',
     6       'EVB(21)  ','EVB(22)  ','EVB(23)  ','EVB(24)  ',
     7       'EVB(25)  ','EVB(26)  ','EVB(27)  ','EVB(28)  ',
     8       'EVB(29)  ','EVB(30)  ','EVB(31)  ','EVB(32)  ',
     9       'EVB(33)  ','EVB(34)  ','EVB(35)  ','EVB(36)  ',
     1       'EVB(37)  ','EVB(38)  ','EVB(39)  ','EVB(40)  ',
     2       'EVB(41)  ','EVB(42)  ','EVB(43)  ','EVB(44)  ',
     3       'EVB(45)  ','EVB(46)  ','EVB(47)  ','EVB(48)  ',
     4       'EVB(49)  ','EVB(50)  ','EVB(51)  ','EVB(52)  '/

     DATA LB2/'EVNB(1)  ','EVNB(2)  ','EVNB(3)  ','EVNB(4)  ',
     2       'EVNB(5)  ','EVNB(6)  ','EVNB(7)  ','EVNB(8)  ',
     3       'EVNB(9)  ','EVNB(10) ','EVNB(11) ','EVNB(12) ',
     4       'EVNB(13) ','EVNB(14) ','EVNB(15) ','EVNB(16) ',
     5       'EVNB(17) ','EVNB(18) ','EVNB(19) ','EVNB(20) ',
     6       'EVNB(21) ','EVNB(22) ','EVNB(23) ','EVNB(24) ',
     7       'EVNB(25) ','EVNB(26) ','EVNB(27) ','EVNB(28) ',
     8       'EVNB(29) ','EVNB(30) ','EVNB(31) ','EVNB(32) ',
     9       'EVNB(33) ','EVNB(34) ','EVNB(35) ','EVNB(36) ',
     1       'EVNB(37) ','EVNB(38) ','EVNB(39) ','EVNB(40) ',
     2       'EVNB(41) ','EVNB(42) ','EVNB(43) ','EVNB(44) ',
     3       'EVNB(45) ','EVNB(46) ','EVNB(47) ','EVNB(48) ',
     4       'EVNB(49) ','EVNB(50) ','EVNB(51) ','EVNB(52) '/

C ************************************************************
C
C     INPUT DATA
C
C       CALL UNDFL(LFLAG)

      write(*,1901)
1901    format(' input name for behavior file in a20 format',/)
```

Program GENSEN (cont'd)

```
      read(*,1902)fileb
1902  format(a20)

      write(*,1907)
1907  format(' input name for non-behavior file in a20 format',/)
      read(*,1902)filenb

        write(*,1903)
1903    format(' input name for output file in a20 format',/)
        read(*,1902)fileout

      write(*,1997)
1997  format(' input number of parameters in i2 format',/)
      read(*,107)npar

      write(*,1998)
1998  format(' input mapping control in i2 format',/)
      read(*,107)map

      write(*,1999)
1999  format(' input 1 for full printout, 0 for reduced,',
     1  ' in i2 format',/)
      read(*,107)iprnt

      write(*,1996)
1996  format(' input K-S probability level code for generating',
     1  ' prob. plots',/,' (in i2 format)',//,
     2  ' prob. level:  1.0   .10   .05   .025   .01   .005   .001',/,
     3  '       code:   0     1     2     3     4     5      6',/)
      read(*,107)iprob

      open(unit=13,file=filenb)
      open(unit=12,file=fileb)
      open(unit=11,file=fileout)


      MAPO=MAP
      NOF=1

      DO 907 JK=1,NOF

      MAP=MAPO
      REWIND 12
      REWIND 13
      READ(13,1919)(TITLE(I),I=1,7)
```

Program GENSEN (cont'd)

```
      READ(12,1919)(TITLE(I),I=1,7)
1919   FORMAT(/,7A10)

        WRITE(11,9709)LBB,FILEB,LBNB,FILENB
9709   FORMAT(3X,A10,1X,A20,5X,A10,1X,A20)
C      WRITE(11,9074)(TITLE(I),I=1,7)
      WRITE(11,908)JK

      DO 1921 I=1,5
      READ(13,1920)XYZ
1921   READ(12,1920)XYZ
1920   FORMAT(A10)

      DO 900 I=1,NPAR
      READ(13,1920)XYZ
900    READ(12,1922)LAB(I)
1922   FORMAT(1X,A10)

      J=1

901    READ(12,1924,END=2096)(PSI(J,I),I=1,NPAR)
1924   FORMAT(12X,15F7.0)
      NB(J)=1
      J=J+1
      GO TO 901

2096   READ(13,1924,END=3096)(PSI(J,I),I=1,NPAR)
      NB(J)=0
      J=J+1
      GO TO 2096

3096   N5=J-1

        write(*,1235)npar,n5,map
1235   format(' number of parameters=',i4,/,' number of realizations='
   +  ,i4,/,' map=',i4,/,' ********** computing **********',
   +  ///)

C ***************************************************************************
C
C****** CALCULATE MEANS AND VARIANCES OF RAW DATA
C
      DO 903 I=1,NPAR
      XMEAN(I)=0.
      DO 902 J=1,N5
```

Program GENSEN (cont'd)

```
902    XMEAN(I)=XMEAN(I)+PSI(J,I)
      XMEAN(I)=XMEAN(I)/N5
903    CONTINUE

      DO 905 I=1,NPAR
      VAR(I)=0.0
      DO 906 J=1,N5
906    VAR(I)=VAR(I)+(PSI(J,I)-XMEAN(I))**2
      VAR(I)=VAR(I)/(FLOAT(N5)-1.)
905    CONTINUE

C****** NORMALIZE DATA TO OBSERVED RAW MEANS AND VARIANCES (O-1 RESULT)
C      CALCULATE MEANS AND COVARIANCES OF NORMALIZED DATA FOR BOTH
C         CLASSES (B, NB) AND ALL DATA (BNB)
C
      DO 2 K=1,NPAR
      XMBNB(K)=0.
      XMB(K)=0.
      XMNB(K)=0.
      DO 2 J=1,NPAR
      COVBNB(K,J)=0.0
      COVB(K,J)=0.
2      COVNB(K,J)=0.
      KB=0
      KNB=0

      DO 10 I=1,N5
      IF(NB(I).EQ.0) GO TO 5
      KB=KB+1
      DO 4 K=1,NPAR
      PSI(I,K)=(PSI(I,K)-XMEAN(K))/SQRT(VAR(K))
      XMB(K)=XMB(K)+PSI(I,K)
      XMBNB(K)=XMBNB(K)+PSI(I,K)
4      CONTINUE
      GO TO 10
5      KNB=KNB+1
      DO 6 K=1,NPAR
      PSI(I,K)=(PSI(I,K)-XMEAN(K))/SQRT(VAR(K))
      XMNB(K)=XMNB(K)+PSI(I,K)
      XMBNB(K)=XMBNB(K)+PSI(I,K)
6      CONTINUE
10     CONTINUE

      XKB=KB
      XKNB=KNB
```

Program GENSEN (cont'd)

```
      DO 12 K=1,NPAR
      XMBNB(K)=XMBNB(K)/(XKB+XKNB)
      XMB(K)=XMB(K)/XKB
12     XMNB(K)=XMNB(K)/XKNB

      DO 40 J=1,NPAR
      DO 40 K=1,NPAR
      DO 40 I=1,N5
      COVBNB(J,K)=COVBNB(J,K)+(PSI(I,J)-XMBNB(J))*(PSI(I,K)-XMBNB(K))
      IF(NB(I).EQ.0)GO TO 30
      COVB(J,K)=COVB(J,K)+(PSI(I,J)-XMB(J))*(PSI(I,K)-XMB(K))
      GO TO 40
30     COVNB(J,K)=COVNB(J,K)+(PSI(I,J)-XMNB(J))*(PSI(I,K)-XMNB(K))
40     CONTINUE

      DO 9002 K=1,NPAR
      DO 9002 J=1,NPAR
      COVB(J,K)=COVB(J,K)/(XKB-1.)
      COVNB(J,K)=COVNB(J,K)/(XKNB-1.)
9002   COVBNB(J,K)=COVBNB(J,K)/(XKB+XKNB-1.)

C****** PRINT RAW AND NORMALIZED MEANS AND VARIANCES
C
      WRITE(11,101) NPAR,N5
      WRITE(11,190) KB,KNB
      WRITE(11,9000)
      DO 9001 K=1,NPAR
9001   WRITE(11,210)K,LAB(K),XMEAN(K),XMBNB(K),VAR(K),COVBNB(K,K)
      WRITE(11,200)
      DO 45 K=1,NPAR
45     WRITE(11,210)K,LAB(K),XMB(K),XMNB(K),COVB(K,K),COVNB(K,K)

C****** PRINT NORMALIZED COVARIANCE MATRICES
C
      IF(IPRNT.EQ.1)THEN
      WRITE(11,2300)
      DO 4901 K=1,NPAR
4901   WRITE(11,230)K,(COVB(K,J),J=1,NPAR)
      WRITE(11,2301)
      DO 4902 K=1,NPAR
4902   WRITE(11,230)K,(COVNB(K,J),J=1,NPAR)
      WRITE(11,2303)
      DO 4903 K=1,NPAR
4903   WRITE(11,230)K,(COVBNB(K,J),J=1,NPAR)
      ENDIF
```

Program GENSEN (cont'd)

```
 C****** CALCULATE CORRELATION MATRICES
C
      DO 50 J=1,NPAR
      DO 50 K=1,NPAR
      AA(J,K)=COVB(J,K)/SQRT(COVB(J,J)*COVB(K,K))
      BB(J,K)=COVNB(J,K)/SQRT(COVNB(J,J)*COVNB(K,K))
      CC(J,K)=COVBNB(J,K)/SQRT(COVBNB(J,J)*COVBNB(K,K))
50     CONTINUE

C****** PRINT CORRELATION MATRICES
C
      WRITE(11,220)
      DO 60 K=1,NPAR
60     WRITE(11,230)K,(AA(K,J),J=1,NPAR)
      WRITE(11,240)
      DO 70 K=1,NPAR
70     WRITE(11,230)K,(BB(K,J),J=1,NPAR)
      WRITE(11,241)
      DO 68 K=1,NPAR
68     WRITE(11,230)K,(CC(K,J),J=1,NPAR)

C****** CALCULATE AND PRINT EIGENVECTORS FOR COVARIANCE MATRICES
C
      IF(IPRNT.EQ.1)THEN

      WRITE(11,8001)
      CALL MATCOPY(COVB,NPAR,DD)
      CALL JACOBI(DD,NPAR,52,EVAL,EV,NROT)
        CALL EIGSRT(EVAL,EV,NPAR,52)
      WRITE(11,8003) NROT
      WRITE(11,8004) (EVAL(LL),LL=1,NPAR)
      WRITE(11,8006)
      DO 8222 J=1,NPAR
      WRITE(11,230) J,(EV(J,LL),LL=1,NPAR)
8222   CONTINUE

      WRITE(11,8002)
      CALL MATCOPY(COVNB,NPAR,DD)
      CALL JACOBI(DD,NPAR,52,EVAL,EV,NROT)
        CALL EIGSRT(EVAL,EV,NPAR,52)
      WRITE(11,8003)NROT
      WRITE(11,8004)(EVAL(LL),LL=1,NPAR)
      WRITE(11,8006)
      DO 8033 J=1,NPAR
      WRITE(11,230)J,(EV(J,LL),LL=1,NPAR)
```

Program GENSEN (cont'd)

```
 8033   CONTINUE

      ENDIF

C****** CALCULATE CROSS-PRODUCT OF MEANS MATRICES FOR EACH CLASS
C
      DO 619 I=1,NPAR
      DO 619 K=1,NPAR
      AA(I,K)=XMB(I)*XMB(K)
      BB(I,K)=XMNB(I)*XMNB(K)
619    CONTINUE

C****** PRINT CROSS PRODUCT OF MEANS MATRICES
C
      IF(IPRNT.EQ.1)THEN
      WRITE(11,209)
      DO 620 J=1,NPAR
620    WRITE(11,230) J,(AA(J,K),K=1,NPAR)
      WRITE(11,208)
      DO 621 J=1,NPAR
621    WRITE(11,230)J,(BB(J,K),K=1,NPAR)
      ENDIF

C****** CALCULATE AND PRINT EIGENVECTORS FOR CROSS-PROD OF MEANS
MATRICES
C
      IF(IPRNT.EQ.1)THEN

      WRITE(11,8008)
      CALL MATCOPY(AA,NPAR,DD)
      CALL JACOBI(DD,NPAR,52,EVAL,EV,NROT)
        CALL EIGSRT(EVAL,EV,NPAR,52)
      WRITE(11,8003) NROT
      WRITE(11,8004) (EVAL(LL),LL=1,NPAR)
      WRITE(11,8006)
      DO 8999 J=1,NPAR
      WRITE(11,230) J,(EV(J,LL),LL=1,NPAR)
8999   CONTINUE

      WRITE(11,8009)
      CALL MATCOPY(BB,NPAR,DD)
      CALL JACOBI(DD,NPAR,52,EVAL,EV,NROT)
        CALL EIGSRT(EVAL,EV,NPAR,52)
      WRITE(11,8003)NROT
      WRITE(11,8004)(EVAL(LL),LL=1,NPAR)
```

Program GENSEN (cont'd)

```
      WRITE(11,8006)
      DO 8110 J=1,NPAR
      WRITE(11,230)J,(EV(J,LL),LL=1,NPAR)
8110  CONTINUE

      ENDIF

C****** CALCULATE AND PRINT SUM OF COVAR AND CROSS-PROD MATRICES
C     (F-K MATRICES) FOR EACH CLASS, AND THE WEIGHTED SUM OF
C     THE TWO F-K MATRICES
C
      DO 8121 I=1,NPAR
      DO 8121 K=1,NPAR
      C2(I,K)=COVB(I,K)+AA(I,K)
      C1(I,K)=COVNB(I,K)+BB(I,K)
8121  CONTINUE

      DO 9003 I=1,NPAR
      DO 9003 K=1,NPAR
9003  CT(I,K)=(C1(I,K)*XKNB+C2(I,K)*XKB)/(XKNB+XKB)

      IF(IPRNT.EQ.1)THEN
      WRITE(11,8888)
      DO 8877 K=1,NPAR
8877  WRITE(11,230) K,(C2(K,J),J=1,NPAR)
      WRITE(11,8889)
      DO 8878 K=1,NPAR
8878  WRITE(11,230)K,(C1(K,J),J=1,NPAR)
      WRITE(11,9004)
      DO 9005 K=1,NPAR
9005  WRITE(11,230)K,(CT(K,J),J=1,NPAR)
      ENDIF

C****** CALCULATE AND PRINT EIGENVECTORS, EIGENVALUES AND PRIOR
C     WEIGHTED EIGENVALUES FOR THE F-K MATRICES FOR EACH CLASS
C
      WRITE(11,8010)
      CALL MATCOPY(C2,NPAR,DD)
      CALL JACOBI(DD,NPAR,52,EVAL,EV,NROT)
        CALL EIGSRT(EVAL,EV,NPAR,52)
      WRITE(11,8003)NROT
      WRITE(11,8004) (EVAL(L),L=1,NPAR)
      DO 8866 L=1,NPAR
8866  EVAL(L)=EVAL(L)*XKB/(XKB+XKNB)
      WRITE(11,232)(EVAL(L),L=1,NPAR)
```

Program GENSEN (cont'd)

```
      WRITE(11,8006)
      DO 8011 J=1,NPAR
      WRITE(11,230) J,(EV(J,L),L=1,NPAR)
      EVALB(J)=EVAL(J)
      DO 8011 L=1,NPAR
      EVB(J,L)=EV(J,L)
8011  CONTINUE

      WRITE(11,8111)
      CALL MATCOPY(C1,NPAR,DD)
      CALL JACOBI(DD,NPAR,52,EVAL,EV,NROT)
        CALL EIGSRT(EVAL,EV,NPAR,52)
      WRITE(11,8003)NROT
      WRITE(11,8004)(EVAL(L),L=1,NPAR)
      DO 8867 L=1,NPAR
8867  EVAL(L)=EVAL(L)*XKNB/(XKB+XKNB)
      WRITE(11,232)(EVAL(L),L=1,NPAR)
      WRITE(11,8006)
      DO 8112 J=1,NPAR
      WRITE(11,230)J,(EV(J,L),L=1,NPAR)
8112  CONTINUE

C****** CALCULATE AND PRINT THE SUM OF THE EIGENVALUES FOR EACH CLASS
C
      DO 9090 J=1,NPAR
      K=NPAR-J+1
9090  EVAL(J)=EVAL(J)+EVALB(K)
      WRITE(11,9009)(EVAL(J),J=1,NPAR)

C*************************************************************************
C
C****** ANALYZE DISTRIBUTIONS OF DATA FOR TWO CLASSES
C     ANALYSES ARE FOR RAW DATA (MAP=0) OR TRANSFORMED (MAPPED) DATA
C     USING EGENVECTORS FROM F-K MATRICES (1=B, 2=NB)
C
C     THE DATA ARE STORED IN VMAP WITH OR WITHOUT TRANSFORMATIONS
C
      IF(MAP.EQ.0) GO TO 6502
9010  IF(MAP.GT.2)GO TO 6502

C****** PERFORM MAPPING
C
      IF(MAP.EQ.1)THEN
      DO 9109 I=1,NPAR
9109  LAB(I)=LB1(I)
```

Program GENSEN (cont'd)

```
      ELSE
      DO 9209 I=1,NPAR
9209   LAB(I)=LB2(I)
      ENDIF

        DO 6610 K=1,NPAR
        XMEAN(K)=0.
6610    VAR(K)=0.

      DO 6500 I=1,N5
      DO 6500 K=1,NPAR
      SUM=0.
      DO 6499 L=1,NPAR
      IF(MAP.EQ.1)SUM=SUM+EVB(L,K)*PSI(I,L)
      IF(MAP.EQ.2)SUM=SUM+EV(L,K)*PSI(I,L)
6499   CONTINUE
        XMEAN(K)=XMEAN(K)+SUM
        VAR(K)=VAR(K)+SUM*SUM
6500    VMAP(I,K)=SUM

      DO 6620 K=1,NPAR
      XMEAN(K)=XMEAN(K)/N5
6620   VAR(K)=(VAR(K)-N5*XMEAN(K)*XMEAN(K))/(N5-1)

      DO 6600 I=1,N5
      DO 6600 K=1,NPAR
6600   VMAP(I,K)=(VMAP(I,K)-XMEAN(K))/SQRT(VAR(K))

      IF(MAP.EQ.1)THEN
      WRITE(11,9076)(K,K=1,NPAR)
      ELSE
      WRITE(11,9077)(K,K=1,NPAR)
      ENDIF

C****** CALCULATE CORRELATION MATRIX BETWEEN MAPPED AND UNTRANSFORMED
C       DATA

      DO 9050 J=1,NPAR
      DO 9050 K=1,NPAR
      SX=0.
        SY=0.
        SXY=0.
        SX2=0.
        SY2=0.0
      DO 9060 I=1,N5
```

Program GENSEN (cont'd)

```
      SX=SX+VMAP(I,K)
      SY=SY+PSI(I,J)
      SX2=SX2+VMAP(I,K)**2
      SY2=SY2+PSI(I,J)**2
9060  SXY=SXY+VMAP(I,K)*PSI(I,J)
      S1=(N5*SX2-SX**2)*(N5*SY2-SY**2)
9050  CC(K,J)=(N5*SXY-SX*SY)/SQRT(S1)
      DO 9080 J=1,NPAR
9080  WRITE(11,9075)J,(CC(I,J),I=1,NPAR)
      GO TO 6501

6502  CONTINUE
      DO 6504 I=1,N5
      DO 6504 K=1,NPAR
6504  VMAP(I,K)=PSI(I,K)

6501  CONTINUE

C*************************************************************
C
C***** CALCULATE AND PRINT MANN-WHITNEY AND KOLMOGOROV-SMIRNOV
STATISTICS
C     STEP THROUGH EACH PARAMETER 1 BY 1 (500 LOOP)

C
C***** RANK ORDER THE PARAMETERS
C

      DO 500 K2=1,NPAR
      KC=1
      KD=1

      DO 501 KA=1,N5
      IF(NB(KA).EQ.0) GO TO 102
      A(KC)=VMAP(KA,K2)
      KC=KC+1
      GO TO 501
102   B(KD)=VMAP(KA,K2)
      KD=KD+1
501   CONTINUE
      KC=KC-1
      KD=KD-1

      CALL SORT(KC,A)
      CALL SORT(KD,B)
```

Program GENSEN (cont'd)

```
 C****** RANK ORDERING COMPLETE
C
C*****  MANN-WHITNEY CODE FOR N>20
C      KOLMOGOROV-SMIRNOV TWO SAMPLE TEST
C
      RASUM=0.
      RBSUM=0.
      DAA=0.
      I=1
      J=1
      K=1
      NA=KC
      ANA=NA
      AKD=KD
1010   SNA=(I-1)/ANA
      SNB=(J-1)/AKD
      DA=SNA-SNB
      IF(ABS(DA).GT.DAA) GO TO 211
      GO TO 201
211    DAA=ABS(DA)
      ADA=A(I)
      BDA=B(J)
201    IF(I.GT.NA) GO TO 11
      IF(J.GT.KD) GO TO 712
      IF(B(J)-A(I)) 130,14,13
130    RBSUM=RBSUM+K
      K=K+1
      J=J+1
      GO TO 1010
13     RASUM=RASUM+K
      I=I+1
      K=K+1
      GO TO 1010
14     RASUM=RASUM+K+.5
      RBSUM=RBSUM+K+.5
      I=I+1
      J=J+1
      K=K+2
      GO TO 1010
11     DO 20 KK=J,KD
      RBSUM=RBSUM+K
      K=K+1
20     CONTINUE
      GO TO 22
712    DO 21 KK=1,NA
```

Program GENSEN (cont'd)

```
      RASUM=RASUM+K
      K=K+1
21     CONTINUE
22     ASTAT=NA*KD+NA*(NA+1)/2.-RASUM
      BSTAT=NA*KD+KD*(KD+1)/2.-RBSUM
      USTAT=AMIN1(ASTAT,BSTAT)

C****** ERROR CHECK
C
      BUG=NA*KD-ASTAT-BSTAT
      IF(ABS(BUG).GT.0.5) GO TO 27
      Z=SQRT(NA*KD*(NA+KD+1)/12.)
      Z=(USTAT-(NA*KD/2.))/Z
      GO TO 28
27     Z=10.E10
28     CONTINUE

C****** PRINT MANN-WHITNEY AND K-S MAX DN STATISTICS
C
      WRITE(11,701) K2,LAB(K2)
      WRITE(11,702) RASUM,RBSUM,ASTAT,BSTAT,Z
      SQ=SQRT((ANA+AKD)/(ANA*AKD))
      DO 1938 KK=1,6
1938   D1(KK)=D2(KK)*SQ
      WRITE(11,7011) (D1(KK),KK=1,6)
      WRITE(11,7001) DAA,ADA,BDA
      IF(IPROB.EQ.0)GO TO 1351
      IF(DAA.LT.D1(IPROB))GO TO 500
1351   CONTINUE

C****** CALCULATE  AND PRINT K-S DN VALUES FOR POINTS IN
C      CUMULATIVE PROB SPACE
C
      IF(IPRNT.EQ.1)WRITE(11,399)
      KK=1
      KJ=1
      DO 350 M=1,19
      PROB=.05*M
351    IF(A(KK).GE.UG(M)) GO TO 352
      KK=KK+1
      IF(KK.GT.NA) GO TO 352
      GO TO 351
352    SN1=(KK-1)/ANA
353    IF(B(KJ).GE.UG(M)) GO TO 354
      KJ=KJ+1
```

Program GENSEN (cont'd)

```
      IF(KJ.GT.KD) GO TO 354
      GO TO 353
354     SN2=(KJ-1)/AKD
      DA=SN1-PROB
      DB=SN2-PROB
      DC=SN1-SN2
      IF(IPRNT.EQ.1)WRITE(11,400) UG(M),PROB,SN1,SN2,DA,DB,DC
      SNN1(M)=SN1
      SNN2(M)=SN2
350     CONTINUE
      IF(IPRNT.EQ.1)WRITE(11,9071)
9071    FORMAT(//)

C****** PLOT CUMULATIVE PROB CURVE FOR BOTH CLASSES
C
      DO 909 I=1,100
      LIN(I)=CBL
909     CONTINUE

      WRITE(11,910)LAB(K2)
910     FORMAT(//,1X,'CUMULATIVE PROBABILITY PLOT',3X,A10,
     2 //,9X,'0.0',17X,'0.2',17X,'0.4',17X,'0.6',17X,'0.8',
     2 17X,'1.0',/,10X,10('*.........'),'*')

      DO 911 M=1,19
      MY=SNN1(M)*100
      MX=SNN2(M)*100
      IF(MY.GT.0)LIN(MY)=CBB
      IF(MX.GT.0)LIN(MX)=CNN
      WRITE(11,912)UG(M),(LIN(I),I=1,100)
912     FORMAT(1X,F8.3,' *',100A1)
      IF(MY.GT.0)LIN(MY)=CBL
      IF(MX.GT.0)LIN(MX)=CBL
911     CONTINUE

      WRITE(11,913)
913     FORMAT(10X,10('*.........'),'*')

C****** PLOT PROBABILITY DENSITY HISTOGRAMS FOR EACH CLASS
C
      KK=1
      KJ=1
      DO 920 M=1,49
      PROB=(M-1)*.1-2.4
921     IF(A(KK).GT.PROB)GO TO 922
```

Program GENSEN (cont'd)

```
      KK=KK+1
      IF(KK.GT.NA)GO TO 922
      GO TO 921
922     SNN1(M)=(KK-1)/ANA
923     IF(B(KJ).GT.PROB)GO TO 924
      KJ=KJ+1
      IF(KJ.GT.KD)GO TO 924
      GO TO 923
924     SNN2(M)=(KJ-1)/AKD
920     CONTINUE

      SNN1(50)=1.0
        SNN2(50)=1.0
      DO 925 M=1,49
      SNN1(51-M)=SNN1(51-M)-SNN1(50-M)
      SNN2(51-M)=SNN2(51-M)-SNN2(50-M)
925     CONTINUE

      BMX=0.
        BNMX=0.0
      DO 926 M=1,50
      BMX=AMAX1(BMX,SNN1(M))
      BNMX=AMAX1(BNMX,SNN2(M))
926     CONTINUE

      IF(BMX.GT.BNMX)THEN
      BNMX=BMX
      ELSE
      BMX=BNMX
      ENDIF

      DMX=BMX/15.
      DNMX=BNMX/15.
      WRITE(11,936)
936     FORMAT(/,1X,'PROBABILITY DISTRIBUTION PLOTS',//)

      DO 931 MM=1,15
      YB=BMX-MM*DMX
      YNB=BNMX-MM*DNMX
      DO 930 M=1,50
      LIN(M)=CBL
        LIN(50+M)=CBL
      IF(SNN1(M).GT.YB)LIN(M)=CBB
      IF(SNN2(M).GT.YNB)LIN(M+50)=CNN
930     CONTINUE
```

Program GENSEN (cont'd)

```
      MXM=15-(MM-1)
      IF(MOD(MXM,5).EQ.0)GO TO 932
      WRITE(11,933)(LIN(I),I=1,50),(LIN(I),I=51,100)
933     FORMAT(10X,'.',50A1,10X,'.',50A1)
      GO TO 931
932     YB=YB+DMX
      YNB=YNB+DNMX
      WRITE(11,934)YB,(LIN(I),I=1,50),YNB,(LIN(I),I=51,100)
934     FORMAT(1X,F8.3,' *',50A1,F9.3,' *',50A1)
931     CONTINUE

      WRITE(11,935)
935     FORMAT(2(6X,'0.0 *',6('*.....'),'*.'),/,
     2    2(9X,'-2.4',4X,'-1.6',4X,'-0.8',5X,'0.0',5X,
     2    '0.8',5X,'1.6',5X,'2.4'))
      WRITE(11,9020)
9020    FORMAT(/)

500     CONTINUE

C****** END OF ANALYSIS LOOP
C
C*************************************************

      IF(MAP.LE.2.AND.MAP.EQ.MAPO)GO TO 907

      MAP=MAP-1
      IF(MAP.EQ.3)MAP=1
      IF(MAP.EQ.0)GO TO 907
      GO TO 9010

907     CONTINUE

C*********************************************************************
C
C     FORMATS:
C
100     FORMAT(3I4)
107     FORMAT(I2)
108     FORMAT(A1,/,A1)
9000    FORMAT(/,1X,'FOR ALL VALUES (BEHAVIOR AND NON-BEHAVIOR)',/,
     2  1X,'PARAMETER',5X,'ORIGINAL MEAN',9X,'NORMALIZED MEAN',
     3  9X,'ORIGINAL VARIANCE',9X,'NORMALIZED VARIANCE')
9004    FORMAT(/,1X,'CT MATRIX----SUM OF C1 AND C2 MATRICES',
     2  '  WEIGHTED BY PRIOR PROBABILITIES')
```

Program GENSEN (cont'd)

```
 9006   FORMAT(/,1X,'OBSERVED COVARIANCE MATRIX FOR ALL ',
   2 'NORMALIZED VALUES',/,1X,'(BEHAVIOR AND NON-BEHAVIOR)')
9009   FORMAT(/,1X,'SUM OF EIGENVALUES OF C1 AND C2 MATRICES ',
   2 '(REVERSELY ORDERED)',/,1X,19(F4.2,2X))
908    FORMAT(//,1X,'SENSITIVITY ANALYSIS FOR OBJECTIVE',
   2  ' FUNCTION ',I2)
9074   FORMAT(//,1X,7A10)
9078   FORMAT(7A10)
9070   FORMAT(/,1X,'PARAM',19(5X,I2))
9075   FORMAT(4X,I2,19(2X,F5.2))
9076   FORMAT(//,1X,'CORRELATIONS BETWEEN PARAMETER AND ',
   2 'EIGENVECTOR VALUES FOR THE BEHAVIOR (C2) MATRIX',
   3 //,20X,'EIGENVECTOR',/,' PARAM',19I7)
9077   FORMAT(//,1X,'CORRELATIONS BETWEEN PARAMETER AND ',
   2 'EIGENVECTOR VALUES FOR THE NON-BEHAVIOR (C1)',
   3 ' MATRIX',//,20X,'EIGENVECTOR',/,' PARAM',19I7)
9079   FORMAT(7A10,4I4)
625    FORMAT(10E10.3)
101    FORMAT(/,1X,'PARAMETER STATISTICS(NORMALIZED) FOR ',I2,
   2 ' PARAMETERS AND ',I4,' REPLICATIONS')
624    FORMAT(I2)
698    FORMAT(1X,A5)
190    FORMAT(/,1X,'NO. OF BEHAVIORS=',I4,8X,'NO. OF NON-BEHAVIORS='
   2 ,I4)
200    FORMAT(//,1X,'NORMALIZED',/,
   2 1X,'PARAMETER',2X,'MEAN UNDER BEHAVIOR',2X,'MEAN',
   2 ' UNDER NON-BEHAVIOR',2X,'VARIANCE UNDER BEHAVIOR',2X,
   3 'VARIANCE UNDER NON-BEHAVIOR')
210    FORMAT(1X,I2,1X,A10,1X,F15.3,6X,F15.3,10X,F15.3,8X,F15.3)
2301   FORMAT(/,1X,'COVARIANCE MATRIX FOR NON-BEHAVIOR (NORMALIZED)')
8002   FORMAT(/,1X,'EIGENVALUES AND VECTORS FOR NON-BEHAVIOR',
   2 ' COVARIANCE MATRIX')
208    FORMAT(/,1X,'CROSS PRODUCT OF MEANS FOR NON-BEHAVIOR')
8009   FORMAT(/,1X,'EIGENVALUES AND VECTORS FOR CROSS PRODUCTS',
   2  ' OF MEANS FOR NON-BEHAVIOR')
232    FORMAT(/,1X,'EIGENVALUES TIMES PRIOR PROBABILITIES',/,
   2 1X,10(E9.3,3X),/,1X,9(E9.3,3X))
8889   FORMAT(/,1X,'C1 MATRIX----SUM OF COVARIANCE AND CROSS PRODUCT',
   2 ' OF MEANS MATRICES FOR NON-BEHAVIOR')
8111   FORMAT(/,1X,'EIGENVALUES AND VECTORS FOR C1 MATRIX',
   2  ' (NON-BEHAVIOR)')
2300   FORMAT(/,1X,'COVARIANCE MATRIX FOR BEHAVIOR (NORMALIZED)')
2303   FORMAT(/,1X,'COVARIANCE MATRIX FOR ALL DATA (NORMALIZED)')
8888   FORMAT(/,1X,'C2 MATRIX----SUM OF COVARIANCE AND CROSS PRODUCT OF
   2 MEANS MATRICES FOR BEHAVIOR')
```

Program GENSEN (cont'd)

```
 220   FORMAT(/,1X,'CORRELATION MATRIX FOR BEHAVIOR')
230    FORMAT(1X,I2,19(2X,F5.2))
240    FORMAT(/,1X,'CORRELATION MATRIX FOR NON-BEHAVIOR')
241    FORMAT(/,1X,'CORRELATION MATRIX FOR ALL DATA')
8001   FORMAT(/,1X,'EIGENVALUES AND VECTORS FOR BEHAVIOR',
   2  ' COVARIANCE MATRIX')
8003   FORMAT(/,1X,'EIGENVALUES----------',2X,'NROT= ',I4)
8004   FORMAT(1X,10(E9.3,3X)/1X,9(E9.3,3X))
8006   FORMAT(/,1X,'EIGENVECTOR MATRIX----------')
622    FORMAT(1X,1X,19(5X,I2))
209    FORMAT(/,1X,'CROSS PRODUCTS OF MEANS FOR BEHAVIOR')
8008   FORMAT(/,1X,'EIGENVALUES AND VECTORS FOR CROSS PRODUCTS',
   2  ' OF MEANS FOR BEHAVIOR')
8010   FORMAT(/,1X,'EIGENVALUES AND VECTORS FOR C2 MATRIX',
   2   ' (BEHAVIOR)')
701    FORMAT(//,1X,'MANN-WHITNEY U STATISTIC FOR PARAMETER',
   2  1X,I2,1X,'- ',A10)
7001   FORMAT(1X,'DAA=',E15.8,2X,'ADA=',E15.8,2X,'BDA=',E15.8)
702    FORMAT(1X,'RASUM=',E10.3,2X,'RBSUM=',E10.3,
   2  2X,'ASTAT=',E10.3,2X,'BSTAT=',E10.3,2X,'Z=',E10.3)
7011   FORMAT(/,1X,'KOLMOGOROV-SMIRNOV DN STATISTIC.   CRITICAL',
   2  'DN FOR P=.1,.05,.025,.01,.005,.001=',6(2X,F7.3))
399    FORMAT(1X,8X,'U',10X,'PROB',10X,'SNB',10X,'SNNB',9X,'DELB',
   2  9X,'DELNB',8X,'DELBNB')
400    FORMAT(1X,7(F10.3,3X))
C*******************************************************************************

       STOP
       END

       SUBROUTINE MATCOPY(A,N,B)
C   COPY MATRIX A ONTO MATRIX B
       DIMENSION A(52,52),B(52,52)
       DO 30 I=1,52
         DO 30 J=1,52
       IF(I.GT.N.OR.J.GT.N)THEN
       B(I,J)=0.
       ELSE
         B(I,J)=A(I,J)
         ENDIF
30       CONTINUE
         RETURN
         END

     SUBROUTINE EIGSRT(D,V,N,NP)
```

Program GENSEN (cont'd)

```
      DIMENSION D(52),V(52,52)
      DO 13 I=1,N-1
       K=I
       P=D(I)
       DO 11 J=I+1,N
        IF(D(J).GE.P)THEN
         K=J
         P=D(J)
        ENDIF
11     CONTINUE
       IF(K.NE.I)THEN
        D(K)=D(I)
        D(I)=P
        DO 12 J=1,N
         P=V(J,I)
         V(J,I)=V(J,K)
         V(J,K)=P
12      CONTINUE
       ENDIF
13    CONTINUE
      RETURN
      END

      SUBROUTINE JACOBI(A,N,NP,D,V,NROT)
      PARAMETER (NMAX=100)
      DIMENSION A(52,52),D(52),V(52,52),B(NMAX),Z(NMAX)
      DO 12 IP=1,N
       DO 11 IQ=1,N
        V(IP,IQ)=0.
11     CONTINUE
       V(IP,IP)=1.
12    CONTINUE
      DO 13 IP=1,N
       B(IP)=A(IP,IP)
       D(IP)=B(IP)
       Z(IP)=0.
13    CONTINUE
      NROT=0
      DO 24 I=1,50
       SM=0.
       DO 15 IP=1,N-1
        DO 14 IQ=IP+1,N
         SM=SM+ABS(A(IP,IQ))
14      CONTINUE
15     CONTINUE
```

Program GENSEN (cont'd)

```
      IF(SM.EQ.0.)RETURN
      IF(I.LT.4)THEN
       TRESH=0.2*SM/N**2
      ELSE
       TRESH=0.
      ENDIF
      DO 22 IP=1,N-1
       DO 21 IQ=IP+1,N
        G=100.*ABS(A(IP,IQ))
        IF((I.GT.4).AND.(ABS(D(IP))+G.EQ.ABS(D(IP)))
     *     .AND.(ABS(D(IQ))+G.EQ.ABS(D(IQ))))THEN
         A(IP,IQ)=0.
        ELSE IF(ABS(A(IP,IQ)).GT.TRESH)THEN
         H=D(IQ)-D(IP)
         IF(ABS(H)+G.EQ.ABS(H))THEN
          T=A(IP,IQ)/H
         ELSE
          THETA=0.5*H/A(IP,IQ)
          T=1./(ABS(THETA)+SQRT(1.+THETA**2))
          IF(THETA.LT.0.)T=-T
         ENDIF
         C=1./SQRT(1+T**2)
         S=T*C
         TAU=S/(1.+C)
         H=T*A(IP,IQ)
         Z(IP)=Z(IP)-H
         Z(IQ)=Z(IQ)+H
         D(IP)=D(IP)-H
         D(IQ)=D(IQ)+H
         A(IP,IQ)=0.
         DO 16 J=1,IP-1
          G=A(J,IP)
          H=A(J,IQ)
          A(J,IP)=G-S*(H+G*TAU)
          A(J,IQ)=H+S*(G-H*TAU)
16       CONTINUE
         DO 17 J=IP+1,IQ-1
          G=A(IP,J)
          H=A(J,IQ)
          A(IP,J)=G-S*(H+G*TAU)
          A(J,IQ)=H+S*(G-H*TAU)
17       CONTINUE
         DO 18 J=IQ+1,N
          G=A(IP,J)
          H=A(IQ,J)
```

Program GENSEN (cont'd)

```
            A(IP,J)=G-S*(H+G*TAU)
            A(IQ,J)=H+S*(G-H*TAU)
18          CONTINUE
           DO 19 J=1,N
            G=V(J,IP)
            H=V(J,IQ)
            V(J,IP)=G-S*(H+G*TAU)
            V(J,IQ)=H+S*(G-H*TAU)
19          CONTINUE
           NROT=NROT+1
          ENDIF
21        CONTINUE
22      CONTINUE
       DO 23 IP=1,N
        B(IP)=B(IP)+Z(IP)
        D(IP)=B(IP)
        Z(IP)=0.
23      CONTINUE
24    CONTINUE
      PAUSE '50 iterations should never happen'
      RETURN
      END

      SUBROUTINE SORT(N,RA)
      DIMENSION RA(3000)
      L=N/2+1
      IR=N
10    CONTINUE
       IF(L.GT.1)THEN
        L=L-1
        RRA=RA(L)
       ELSE
        RRA=RA(IR)
        RA(IR)=RA(1)
        IR=IR-1
        IF(IR.EQ.1)THEN
         RA(1)=RRA
         RETURN
        ENDIF
       ENDIF
       I=L
       J=L+L
20     IF(J.LE.IR)THEN
        IF(J.LT.IR)THEN
         IF(RA(J).LT.RA(J+1))J=J+1
```

Program GENSEN (cont'd)

```
      ENDIF
      IF(RRA.LT.RA(J))THEN
        RA(I)=RA(J)
        I=J
        J=J+J
      ELSE
        J=IR+1
      ENDIF
    GO TO 20
    ENDIF
    RA(I)=RRA
  GO TO 10
  END
```

APPENDIX D

Table D-1: Output Data from the GENSEN program for Configuration 1

Dose Criteria: 1 mrem/ No Correlated Parameters/ 7 Subareas			
Parameter ID #	**Ranking**	**Parameter Abb.**	**DAA**
40	1	ARDSAVNp	9.64E-01
2	2	MAPM@GM	9.29E-01
47	3	APrs_SAV	9.29E-01
19	4	RD_IV_I	5.84E-01
41	5	ARDSAV_I	4.30E-01
48	6	WPRRG@10	4.22E-01
49	7	WPRRG@20	3.96E-01
17	8	RD_IV_Ra	3.42E-01
52	9	MixZnT20	3.41E-01
3	10	MATI@GM	3.22E-01
45	11	ARDSAVRa	3.09E-01
30	12	SFWt%I7	2.95E-01
28	13	SFWt%I5	2.80E-01
7	14	*Chlorid	2.59E-01
51	15	AqThick5	2.46E-01
44	16	ARDSAVPu	2.38E-01
18	17	RD_IV_Pb	2.20E-01
15	18	RD_IV_Np	2.17E-01
23	19	RD_IV_Nb	2.16E-01
12	20	RD_IV_Pu	2.12E-01
26	21	SFWt%I3	2.12E-01
50	22	PlumeTh5	2.10E-01
10	23	SbArWt%	2.00E-01
8	24	Fow*	1.96E-01
46	25	ARDSAVSe	1.86E-01
16	26	RD_IV_Th	1.85E-01
25	27	SFWt%I2	1.82E-01
43	28	ARDSAV_U	1.66E-01
21	29	RD_IV_Ni	1.65E-01
29	30	SFWt%I6	1.60E-01
32	31	SFWt%C2	1.57E-01
38	32	InvMPerm	1.57E-01
42	33	ARDSAVTc	1.55E-01
20	34	RD_IV_Tc	1.41E-01
24	35	SFWt%I1	1.40E-01
13	36	RD_IV_U	1.39E-01
27	37	SFWt%I4	1.38E-01
33	38	SFWt%C3	1.38E-01
11	39	WP-Def%	1.37E-01
36	40	SFWt%C6	1.37E-01
37	41	SFWt%C7	1.37E-01
9	42	Fmult*	1.36E-01
35	43	SFWt%C5	1.35E-01
31	44	SFWt%C1	1.32E-01
1	45	AAMAI@S	1.29E-01
22	46	RD_IV_Se	1.21E-01
4	47	FOC-R	1.16E-01
34	48	SFWt%C4	1.12E-01
39	49	ARDSAVAm	1.12E-01
5	50	FOCTR	1.05E-01
14	51	RD_IV_Am	7.96E-02
6	52	FOCTR-R	7.60E-02

** DAA -- Maximum Vertical Distance Between The Distribution Under Behavior and the Distribution Under Non-Behavior

Table D-2: Output Data from the GENSEN program for Configuration 2

Dose Criteria: 0.2 mrem/ No Correlated Parameters/ 7 Subareas			
Parameter ID #	**Ranking**	**Parameter Abbreviation**	**DAA**
10	1	SbArWt%	5.42E-01
49	2	WPRRG@20	3.43E-01
2	3	MAPM@GM	3.33E-01
47	4	APrs_SAV	3.33E-01
41	5	ARDSAV_I	2.57E-01
40	6	ARDSAVNp	2.52E-01
35	7	SFWt%C5	1.75E-01
32	8	SFWt%C2	1.75E-01
19	9	RD_IV_I	1.48E-01
48	10	WPRRG@10	1.47E-01
15	11	RD_IV_Np	1.42E-01
52	12	MixZnT20	1.40E-01
8	13	Fow*	1.38E-01
3	14	MATI@GM	1.32E-01
7	15	*Chlorid	1.32E-01
46	16	ARDSAVSe	1.28E-01
36	17	SFWt%C6	1.25E-01
9	18	Fmult*	1.23E-01
23	19	RD_IV_Nb	1.17E-01
22	20	RD_IV_Se	1.10E-01
30	21	SFWt%I7	1.07E-01
42	22	ARDSAVTc	1.03E-01
31	23	SFWt%C1	1.00E-01
44	24	ARDSAVPu	9.83E-02
45	25	ARDSAVRa	9.67E-02
17	26	RD_IV_Ra	9.33E-02
16	27	RD_IV_Th	9.00E-02
25	28	SFWt%I2	9.00E-02
28	29	SFWt%I5	9.00E-02
12	30	RD_IV_Pu	8.33E-02
27	31	SFWt%I4	8.33E-02
34	32	SFWt%C4	8.33E-02
51	33	AqThick5	8.17E-02
11	34	WP-Def%	8.17E-02
37	35	SFWt%C7	7.67E-02
21	36	RD_IV_Ni	7.17E-02
39	37	ARDSAVAm	7.17E-02
5	38	FOCTR	6.67E-02
18	39	RD_IV_Pb	6.67E-02
20	40	RD_IV_Tc	6.67E-02
50	41	PlumeTh5	6.17E-02
1	42	AAMAI@S	6.00E-02
43	43	ARDSAV_U	6.00E-02
33	44	SFWt%C3	5.83E-02
14	45	RD_IV_Am	5.83E-02
6	46	FOCTR-R	5.67E-02
38	47	InvMPerm	5.67E-02
4	48	FOC-R	5.33E-02
29	49	SFWt%I6	5.33E-02
24	50	SFWt%I1	5.00E-02
13	51	RD_IV_U	4.67E-02
26	52	SFWt%I3	4.50E-02

** DAA -- Maximum Vertical Distance Between the Distribution Under Behavior and the Distribution Under Non-Behavior

Table D-3: Output Data from the GENSEN program for Configuration 3

Dose Criteria: 0.2 mrem/ Correlated Input Parameters/ 7 Subareas			
Parameter ID #	**Ranking**	**Parameter Abbreviation**	**DAA**
10	1	SbArWt%	6.11E-01
1	2	AAMAI@S	3.79E-01
49	3	WPRRG@20	3.65E-01
2	4	MAPM@GM	3.28E-01
47	5	APrs_SAV	3.28E-01
8	6	Fow*	2.00E-01
44	7	ARDSAVPu	2.00E-01
39	8	ARDSAVAm	1.94E-01
40	9	ARDSAVNp	1.94E-01
41	10	ARDSAV_I	1.91E-01
33	11	SFWt%C3	1.71E-01
32	12	SFWt%C2	1.61E-01
52	13	MixZnT20	1.51E-01
35	14	SFWt%C5	1.39E-01
43	15	ARDSAV_U	1.33E-01
19	16	RD_IV_I	1.30E-01
23	17	RD_IV_Nb	1.28E-01
48	18	WPRRG@10	1.26E-01
30	19	SFWt%I7	1.08E-01
18	20	RD_IV_Pb	1.07E-01
5	21	FOCTR	1.06E-01
31	22	SFWt%C1	1.04E-01
9	23	Fmult*	9.97E-02
36	24	SFWt%C6	9.53E-02
20	25	RD_IV_Tc	9.52E-02
7	26	*Chlorid	9.50E-02
22	27	RD_IV_Se	9.13E-02
3	28	MATI@GM	8.77E-02
51	29	AqThick5	8.45E-02
4	30	FOC-R	8.25E-02
15	31	RD_IV_Np	8.17E-02
45	32	ARDSAVRa	8.04E-02
12	33	RD_IV_Pu	7.98E-02
26	34	SFWt%I3	7.97E-02
42	35	ARDSAVTc	7.95E-02
34	36	SFWt%C4	7.86E-02
17	37	RD_IV_Ra	7.51E-02
29	38	SFWt%I6	6.89E-02
38	39	InvMPerm	6.73E-02
11	40	WP-Def%	6.72E-02
21	41	RD_IV_Ni	6.42E-02
16	42	RD_IV_Th	6.09E-02
46	43	ARDSAVSe	6.04E-02
13	44	RD_IV_U	5.81E-02
27	45	SFWt%I4	5.56E-02
24	46	SFWt%I1	5.55E-02
50	47	PlumeTh5	5.09E-02
14	48	RD_IV_Am	5.03E-02
37	49	SFWt%C7	4.62E-02
6	50	FOCTR-R	4.60E-02
25	51	SFWt%I2	4.39E-02
28	52	SFWt%I5	4.06E-02

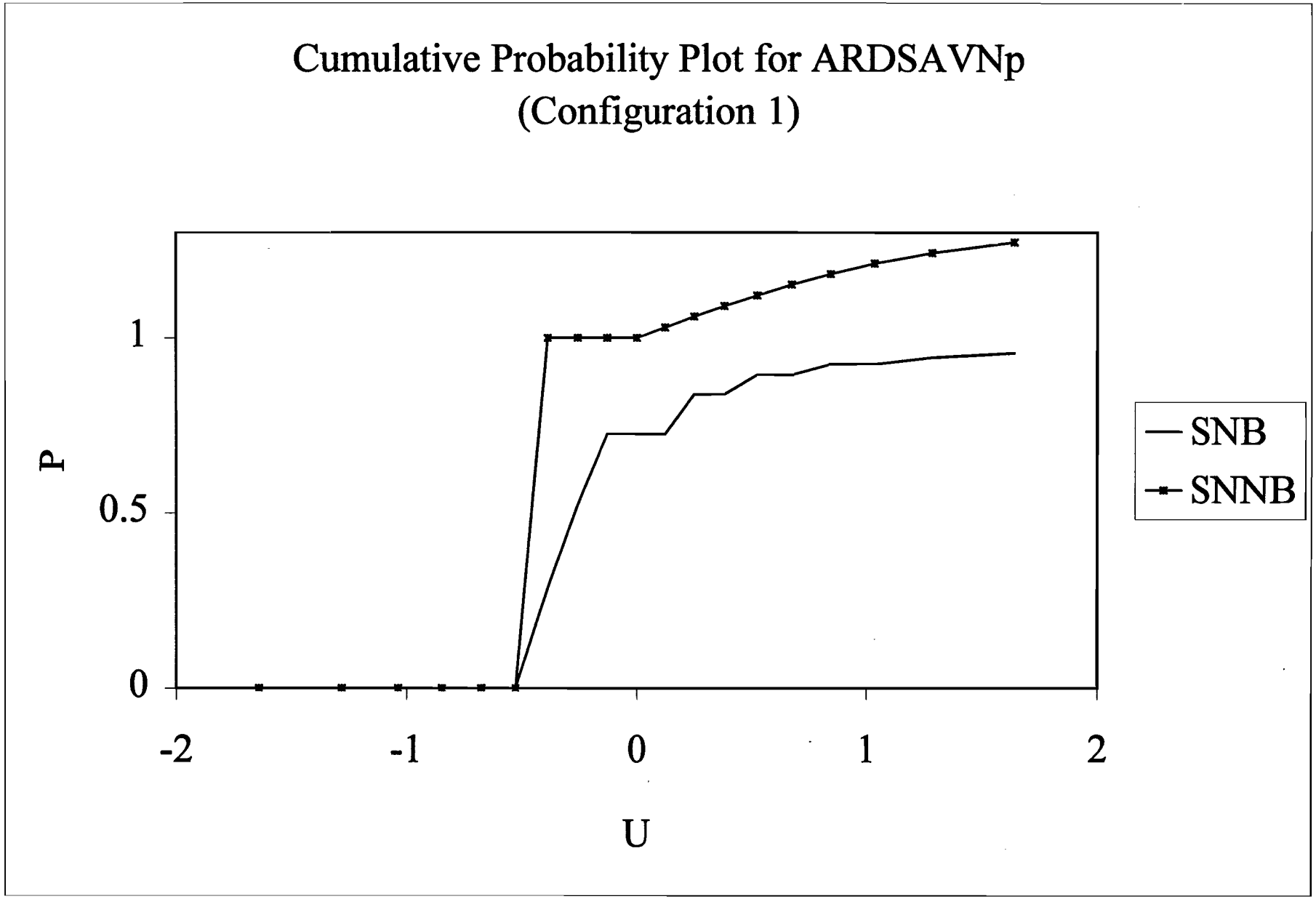
** DAA -- Maximum Vertical Distance Between the Distribution Under Behavior and the Distribution Under Non-Behavior

Table D-4: Output Data from the GENSEN program for Configuration 3

Dose Criteria: 0.2 mrem/ Correlated Parameters/ 7 Subareas			
Parameter ID #	Ranking	Parameter Abbreviation	DAA
1	1	SFWt%C1	0.46187103
26	2	SbArWt%	0.43730348
11	3	AAMAI@S	0.27286422
2	4	MAPM@GM	0.2638889
36	5	APrs_SAV	0.2638889
37	6	WPRRG@20	0.25694442
30	7	ARDSAV_I	0.19542712
9	8	Fow*	0.15421909
40	9	MixZnT20	0.13541669
33	10	ARDSAVPu	0.11170071
29	11	ARDSAVNp	0.10776991
8	12	*Chlorid	0.10547692
32	13	ARDSAV_U	0.10521489
12	14	WP-Def%	0.095322341
7	15	AA_2_1	0.094732702
10	16	Fmult*	0.094536126
14	17	RD_IV_U	0.093881071
28	18	ARDSAVAm	0.093422413
39	19	AqThick5	0.092636287
6	20	FOCTR-R	0.089557111
20	21	RD_IV_I	0.087460697
13	22	RD_IV_Pu	0.084316015
38	23	PlumeTh5	0.078878433
34	24	ARDSAVRa	0.074751019
27	25	InvMPerm	0.074554503
25	26	SFWt%I1	0.073702827
19	27	RD_IV_Pb	0.072785646
16	28	RD_IV_Np	0.071671903
31	29	ARDSAVTc	0.070230618
17	30	RD_IV_Th	0.069444418
22	31	RD_IV_Ni	0.068592727
18	32	RD_IV_Ra	0.067151427
21	33	RD_IV_Tc	0.064006805
24	34	RD_IV_Nb	0.062172413
4	35	FOC-R	0.060731113
23	36	RD_IV_Se	0.058110595
35	37	ARDSAVSe	0.054900408
3	38	MATI@GM	0.053066045
5	39	FOCTR	0.052410901
15	40	RD_IV_Am	0.041273594

** DAA -- Maximum Vertical Distance Between the Distribution Under Behavior and the Distribution Under Non-Behavior

APPENDIX E


Cumulative Probability Plot for ARDSAVNp
(Configuration 1)
P
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0.5
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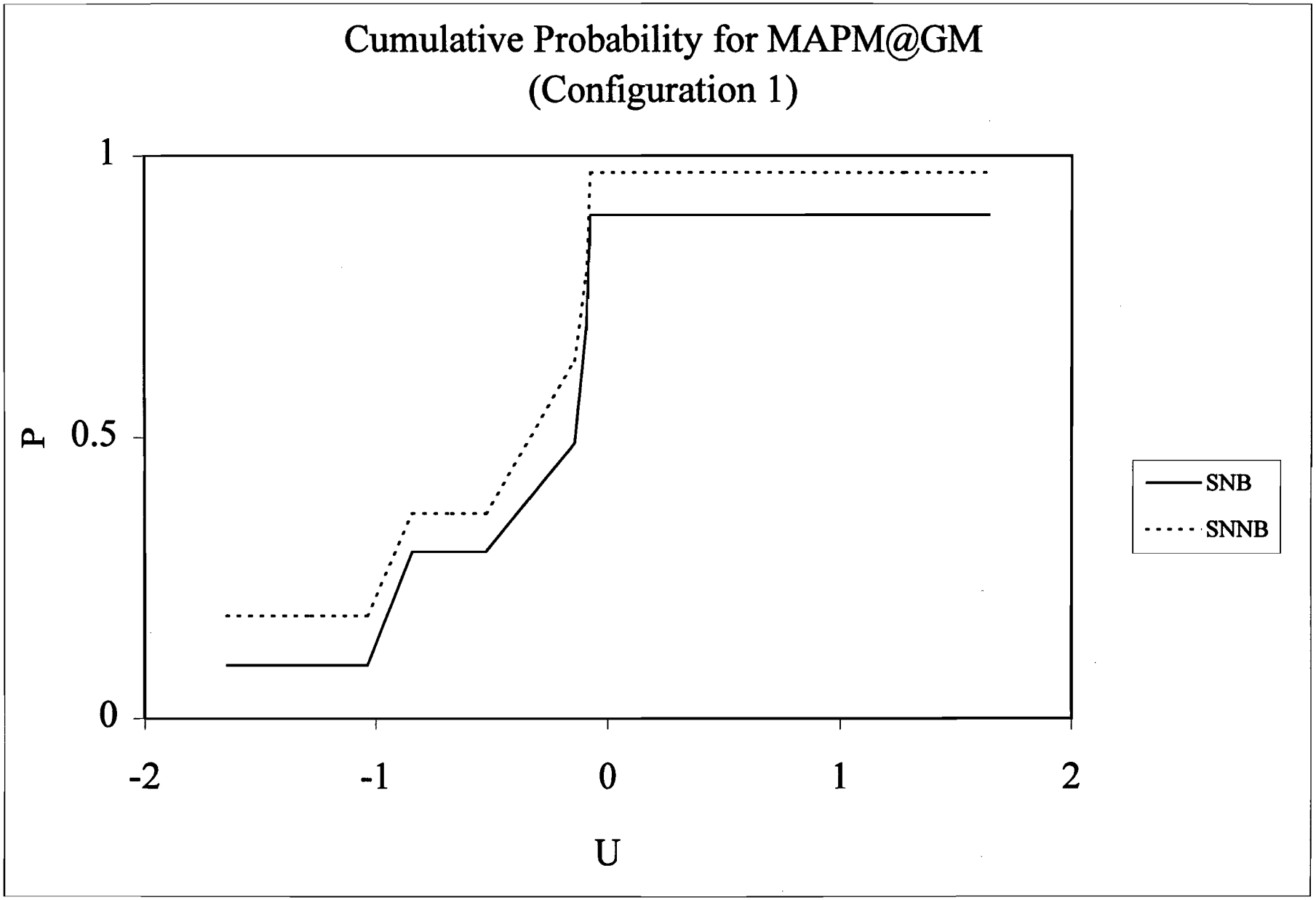
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability for MAPM@GM
(Configuration 1)
1
P 0.5
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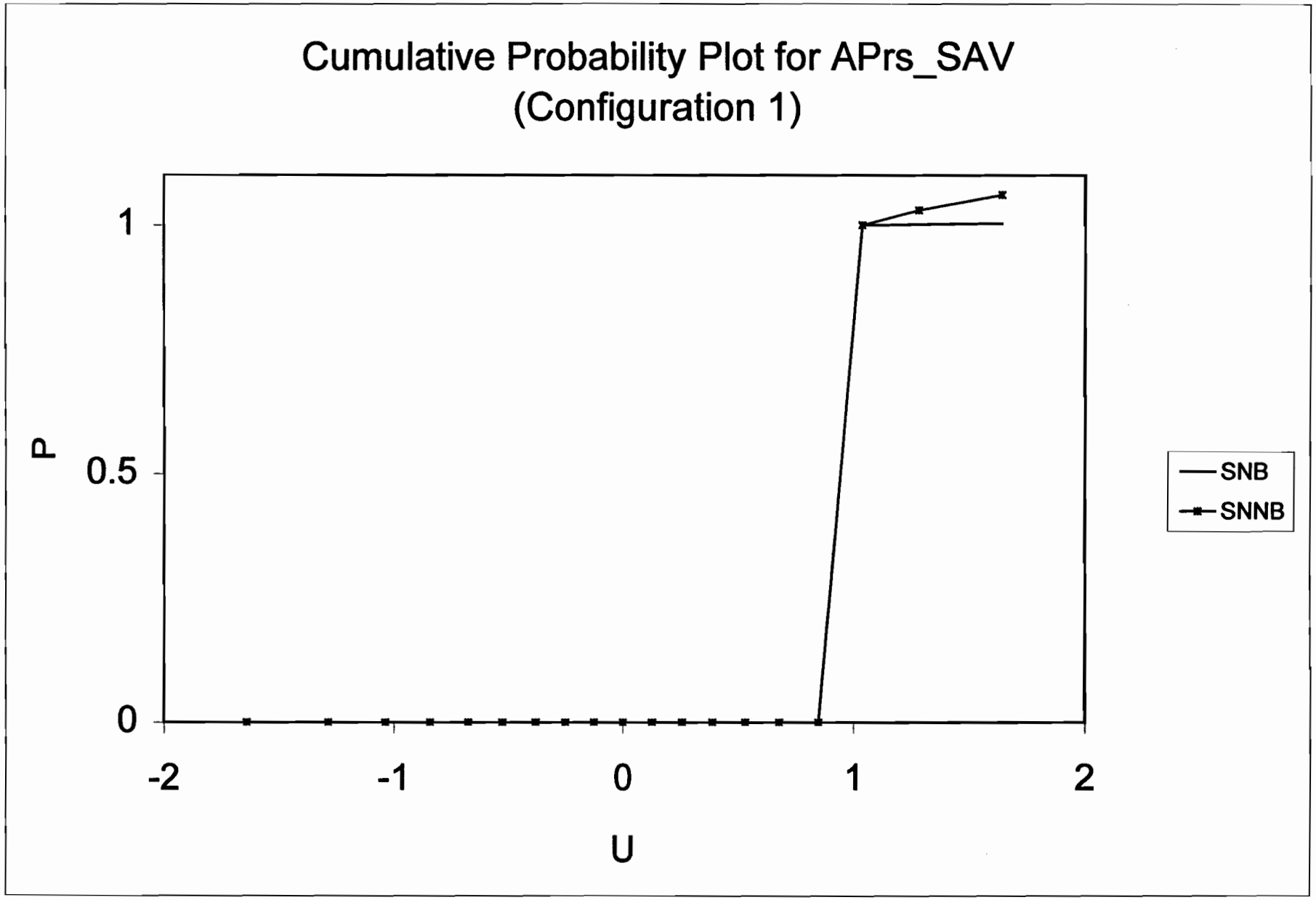
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for APrs_SAV
(Configuration 1)
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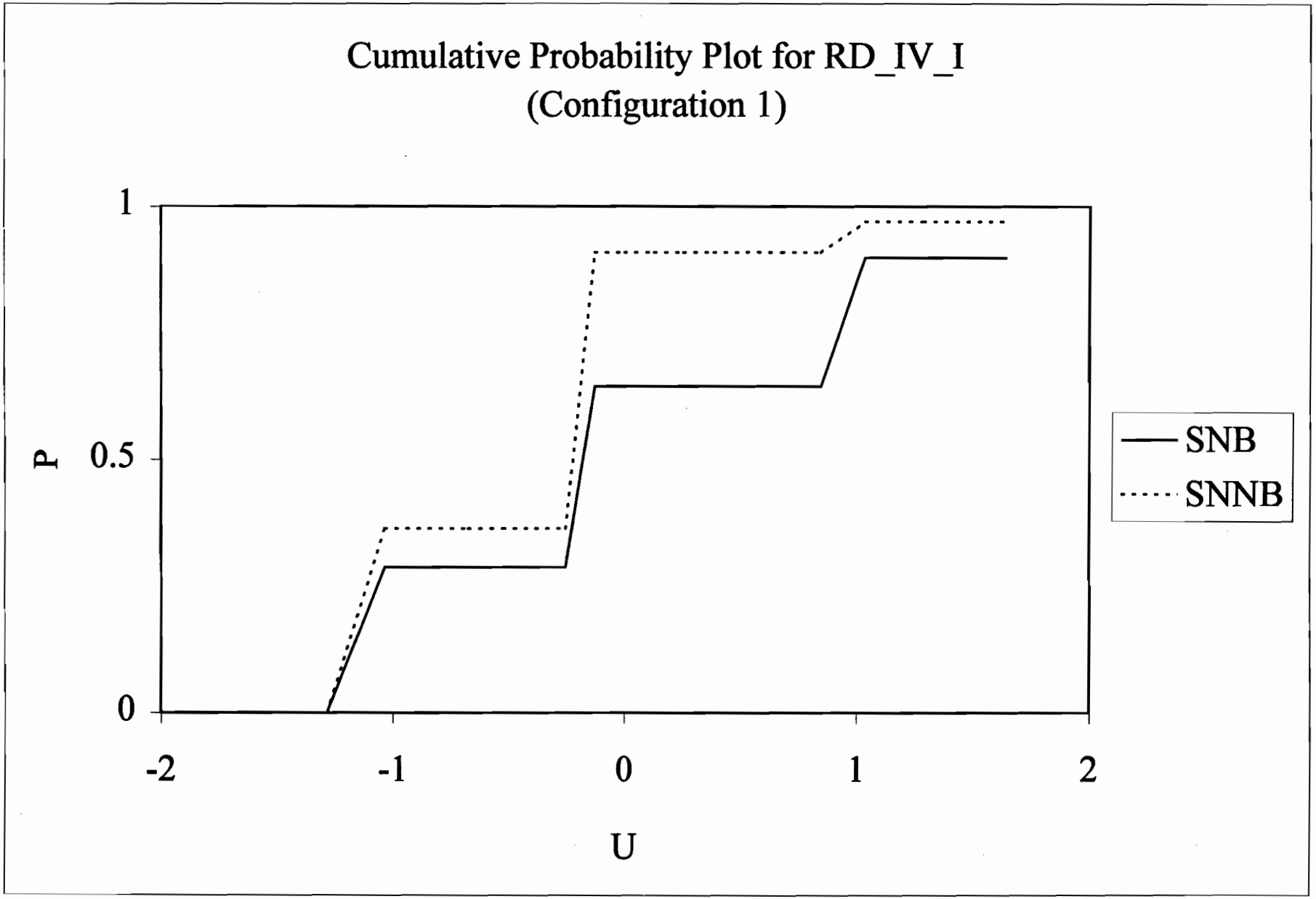
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for RD_IV_I
(Configuration 1)
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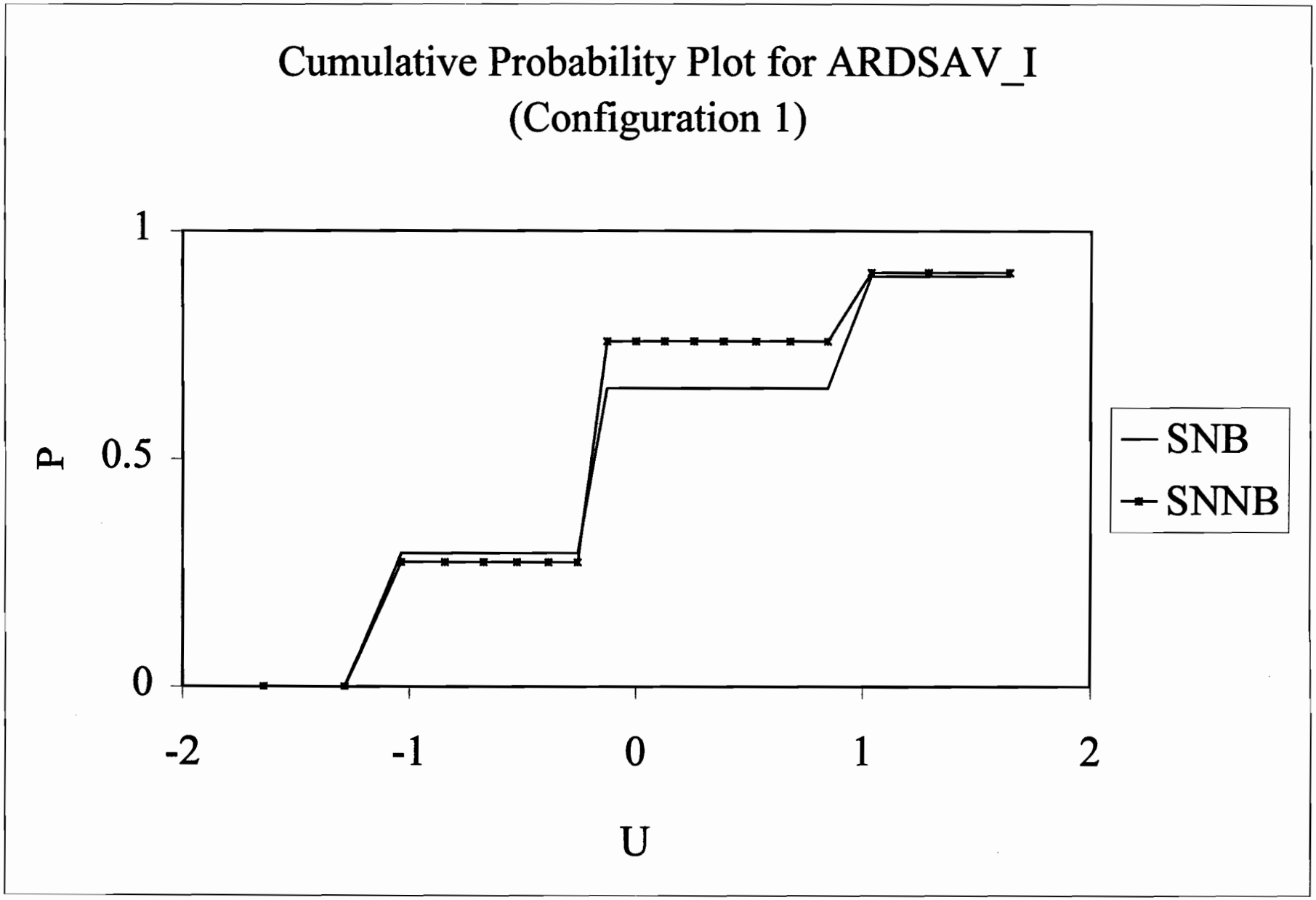
0
P
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for ARDSAV_I
(Configuration 1)
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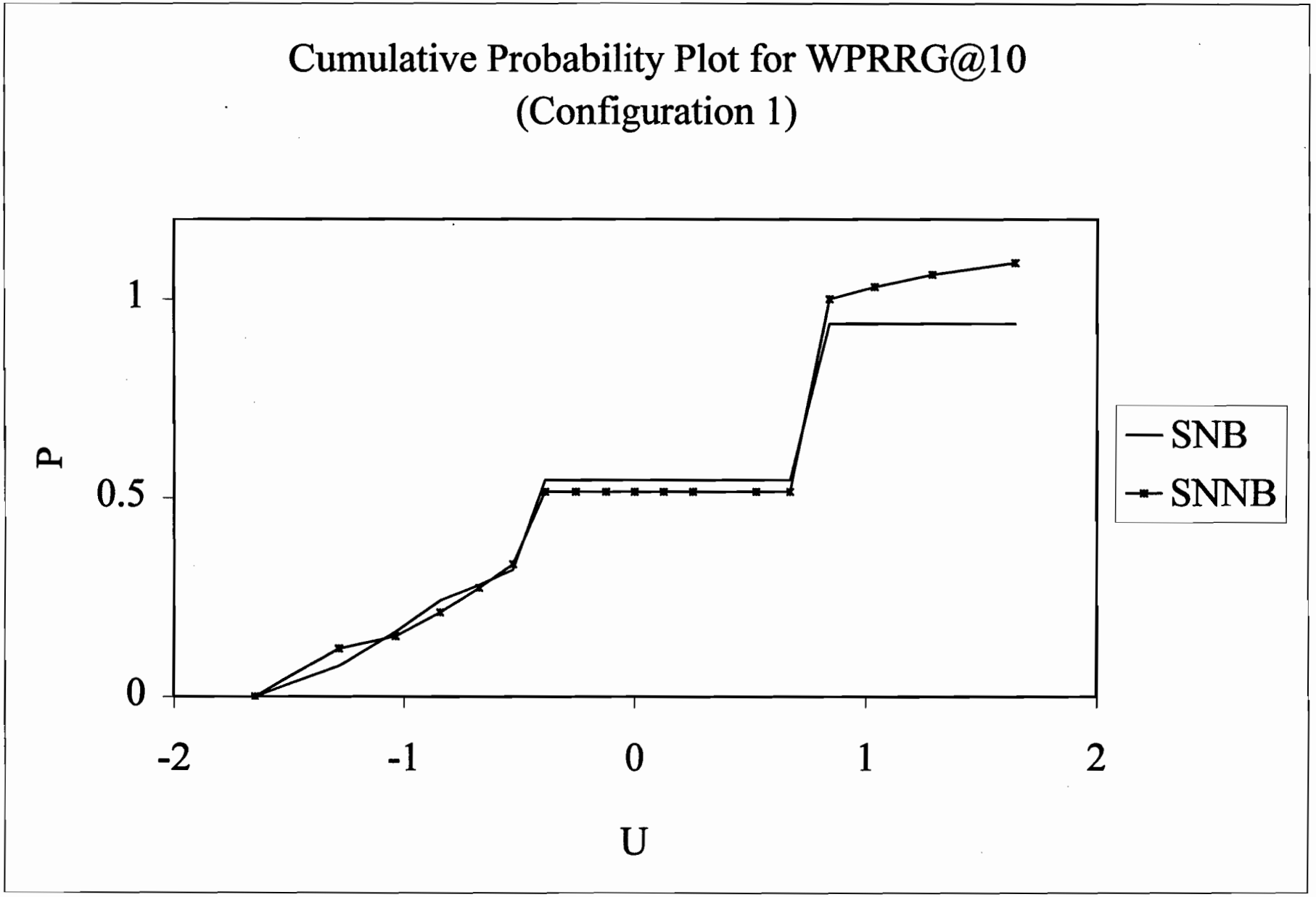
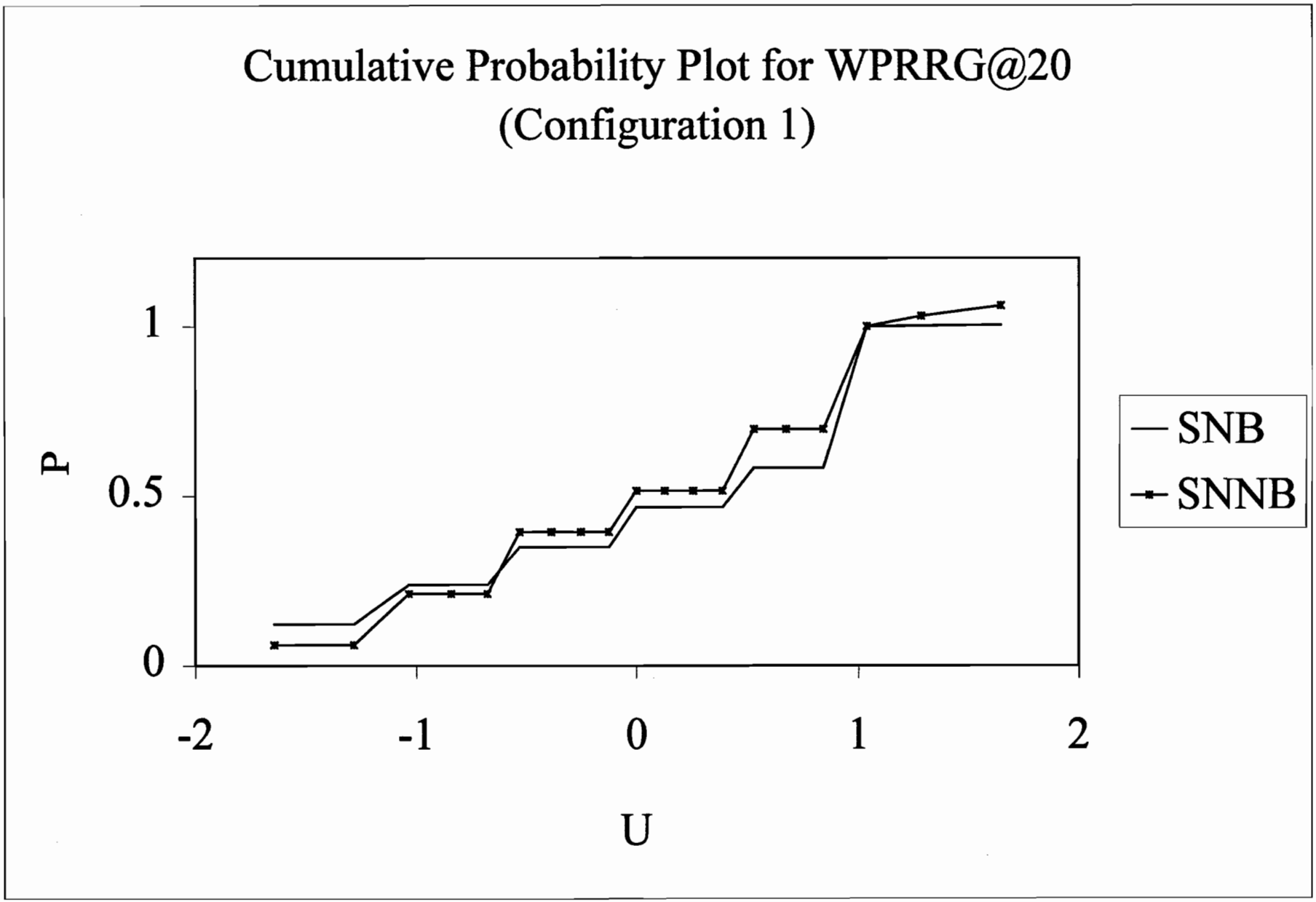
0.5
0
P
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for WPRRG@10
(Configuration 1)
P
1
0.5
0
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for WPRRG@20
(Configuration 1)
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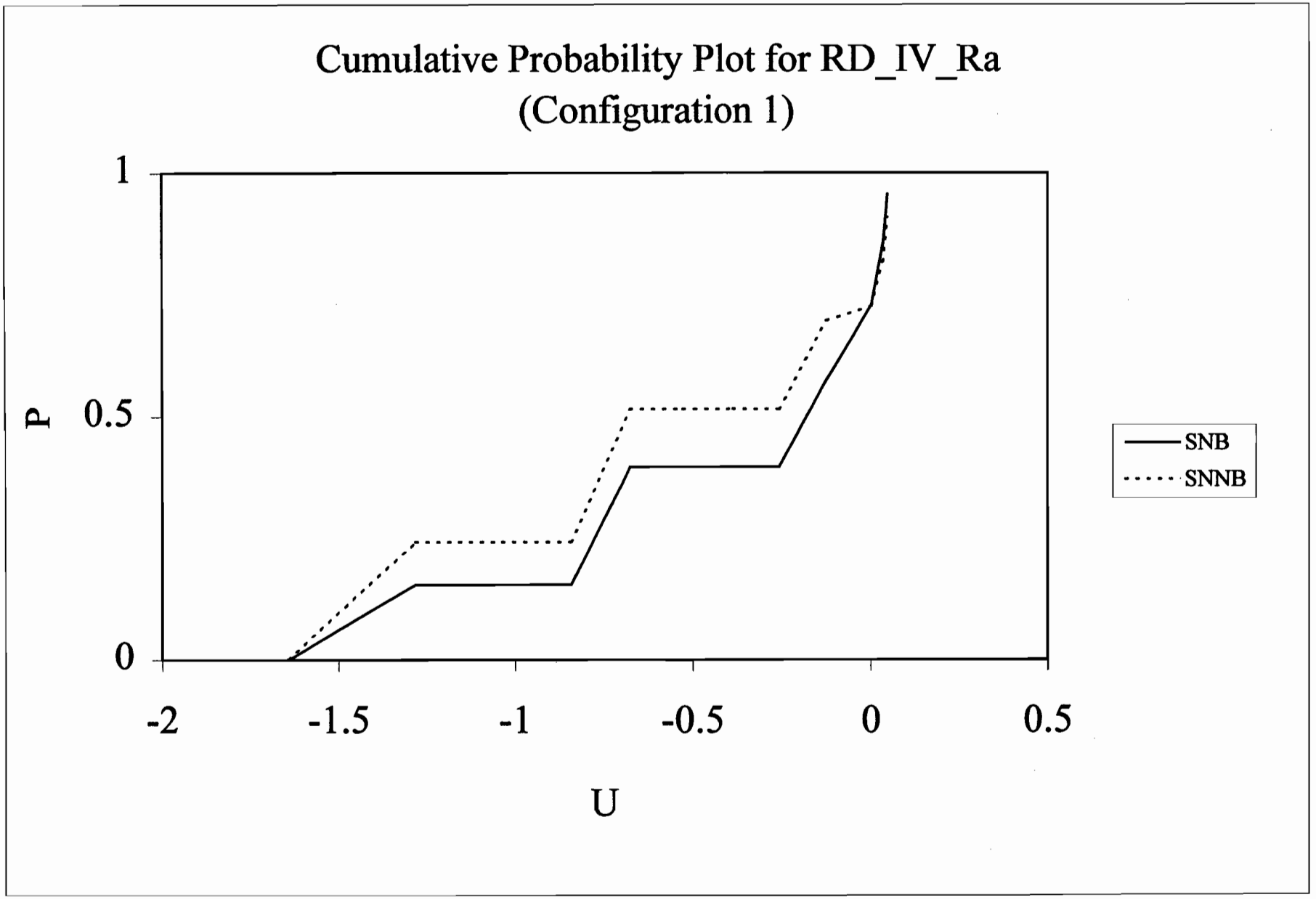
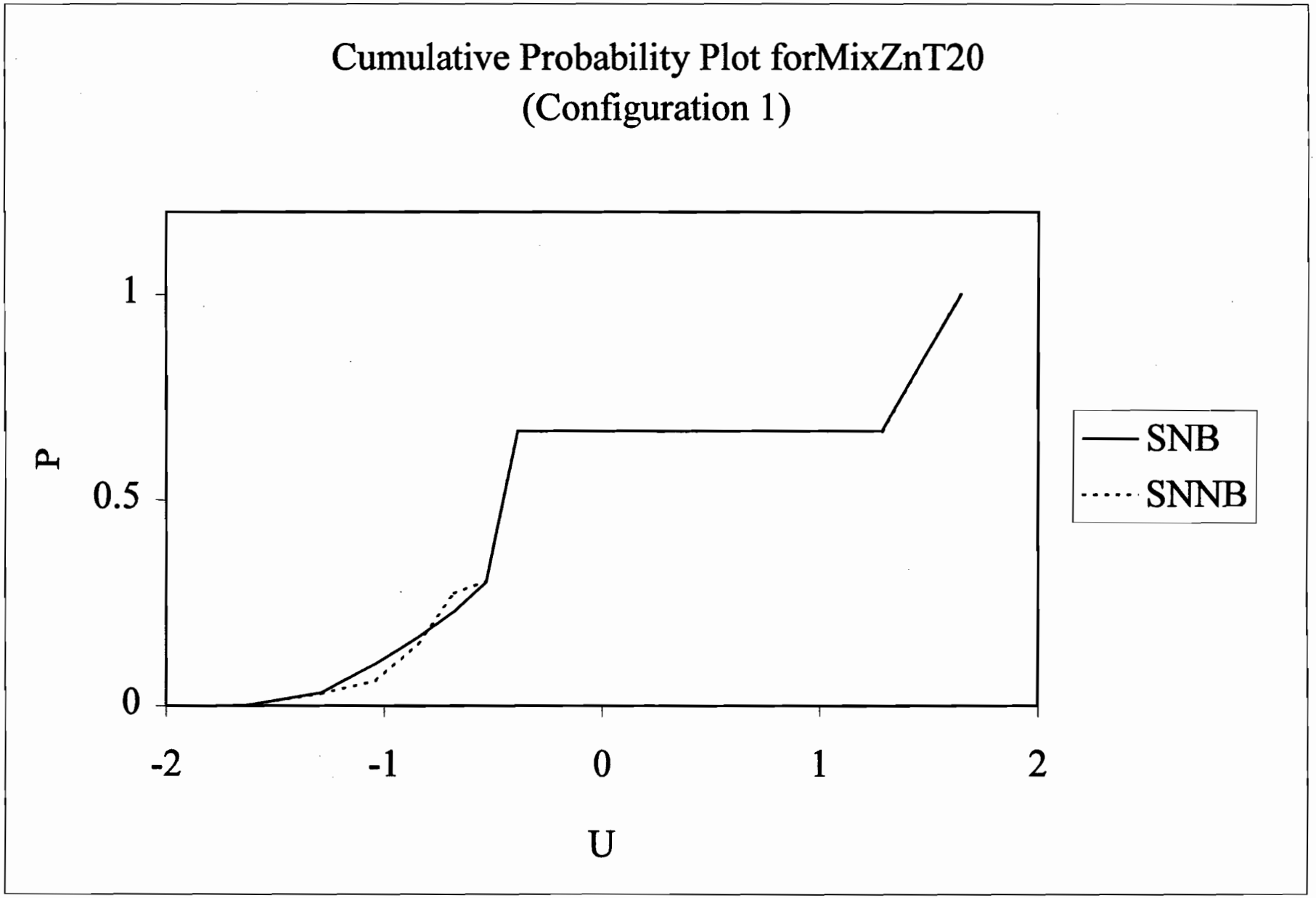
0.5
0
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for RD_IV_Ra
(Configuration 1)
1
P 0.5
0
-2
-1.5
-1
-0.5
0
0.5
U
SNB
SNNB


Cumulative Probability Plot forMixZnT20
(Configuration 1)
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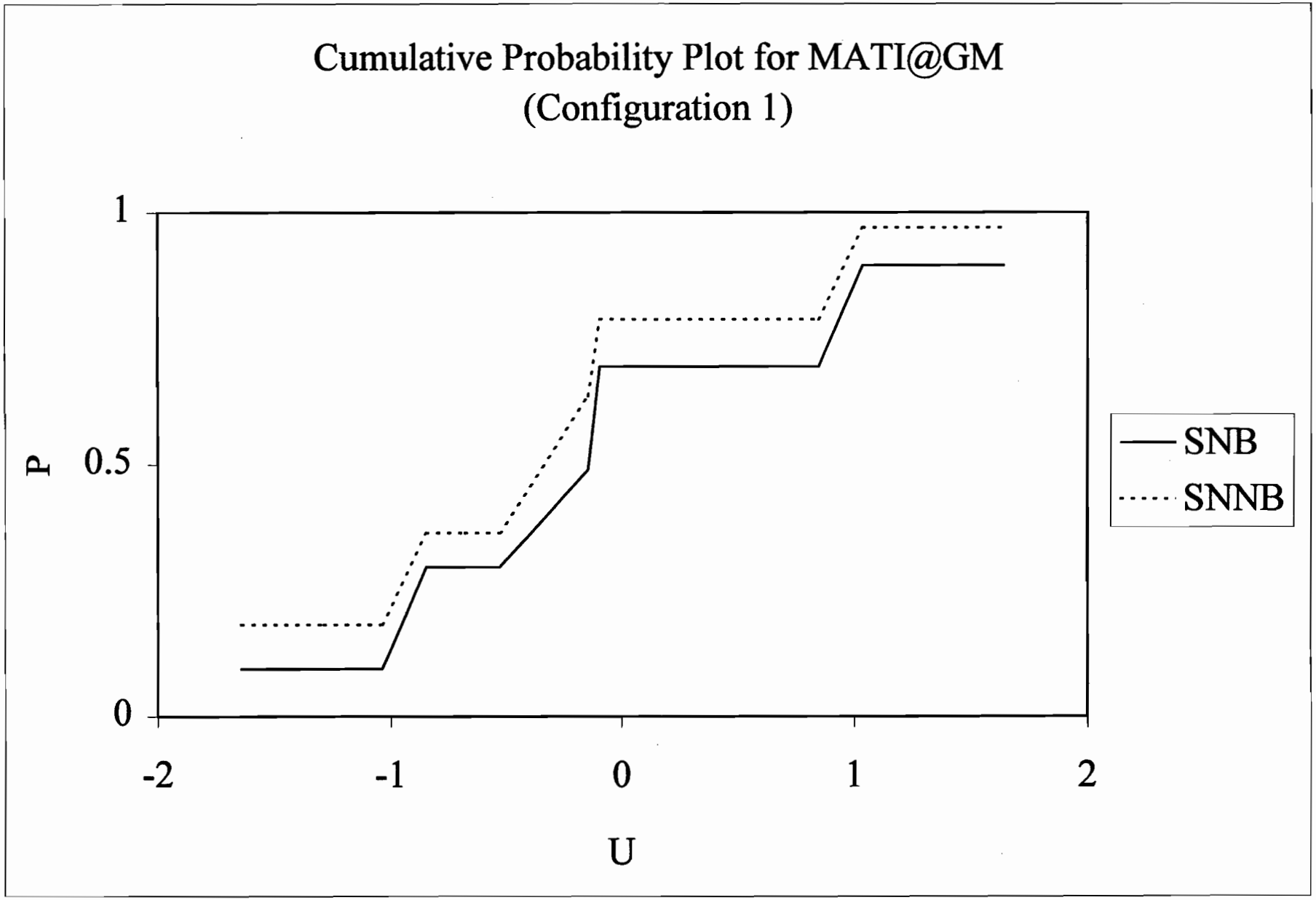
0.5
0
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for MATI@GM
(Configuration 1)
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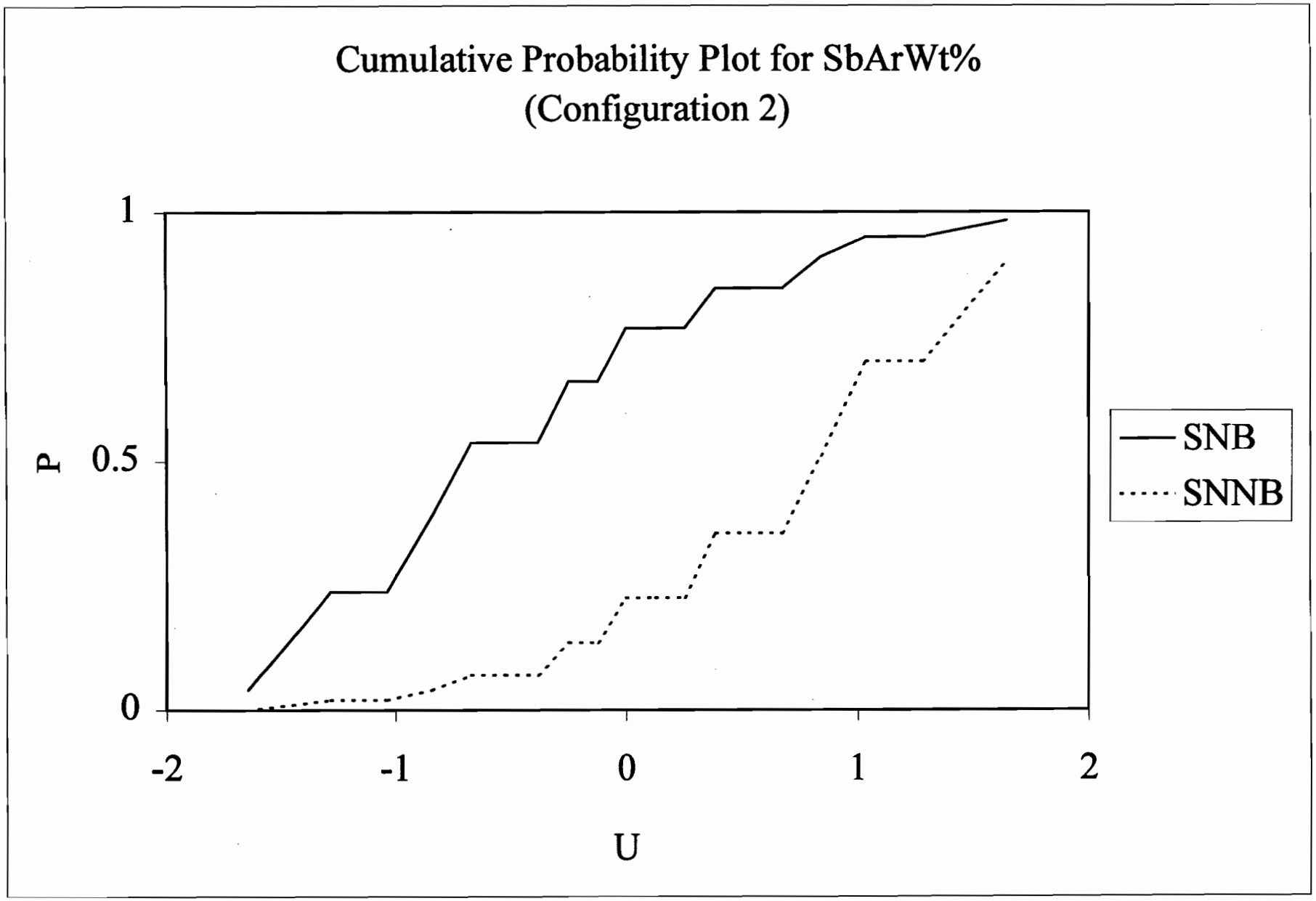
0
P
-2
-1
0
1
2
U
SNB
SNNB

APPENDIX F


Cumulative Probability Plot for SbArWt%
(Configuration 2)
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0.5
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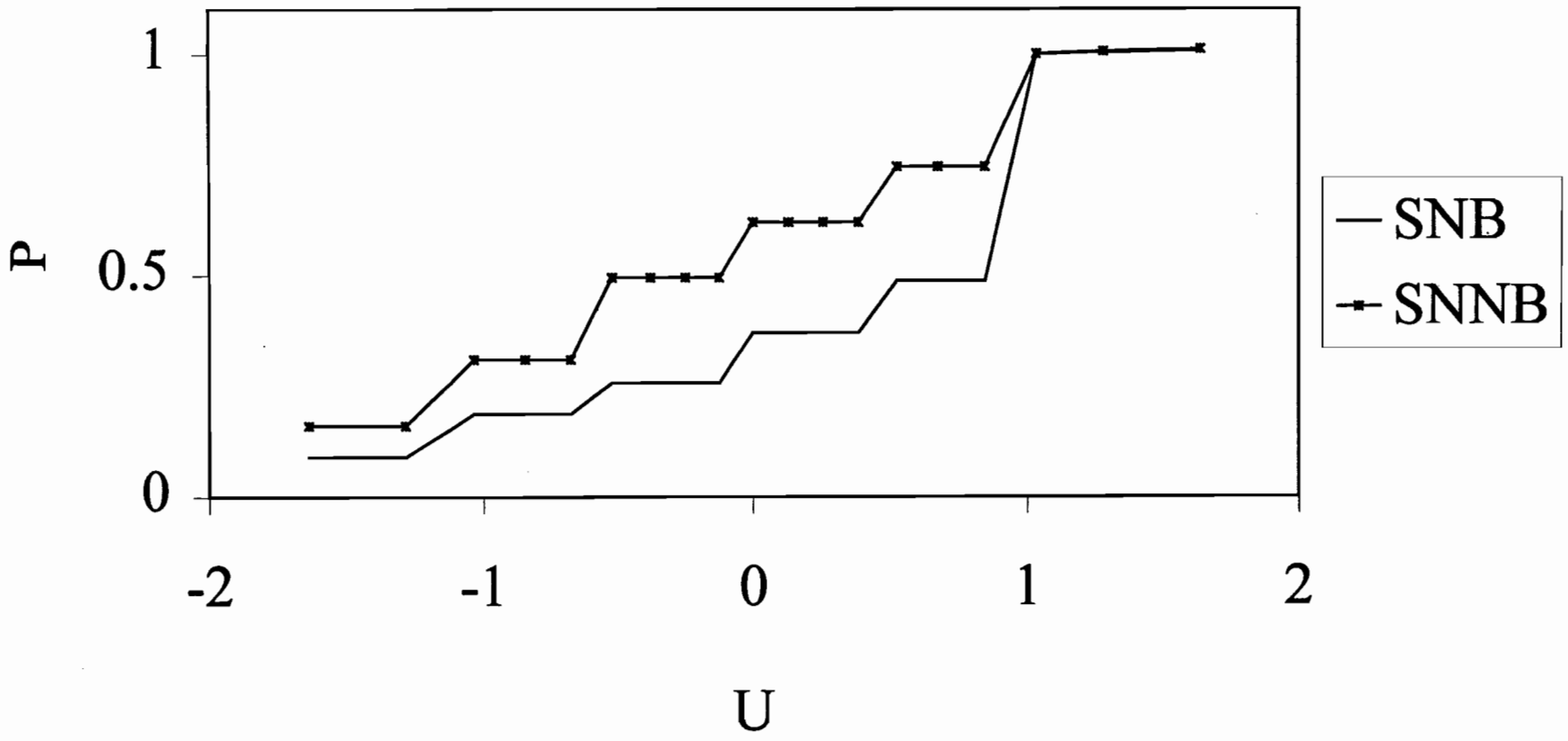
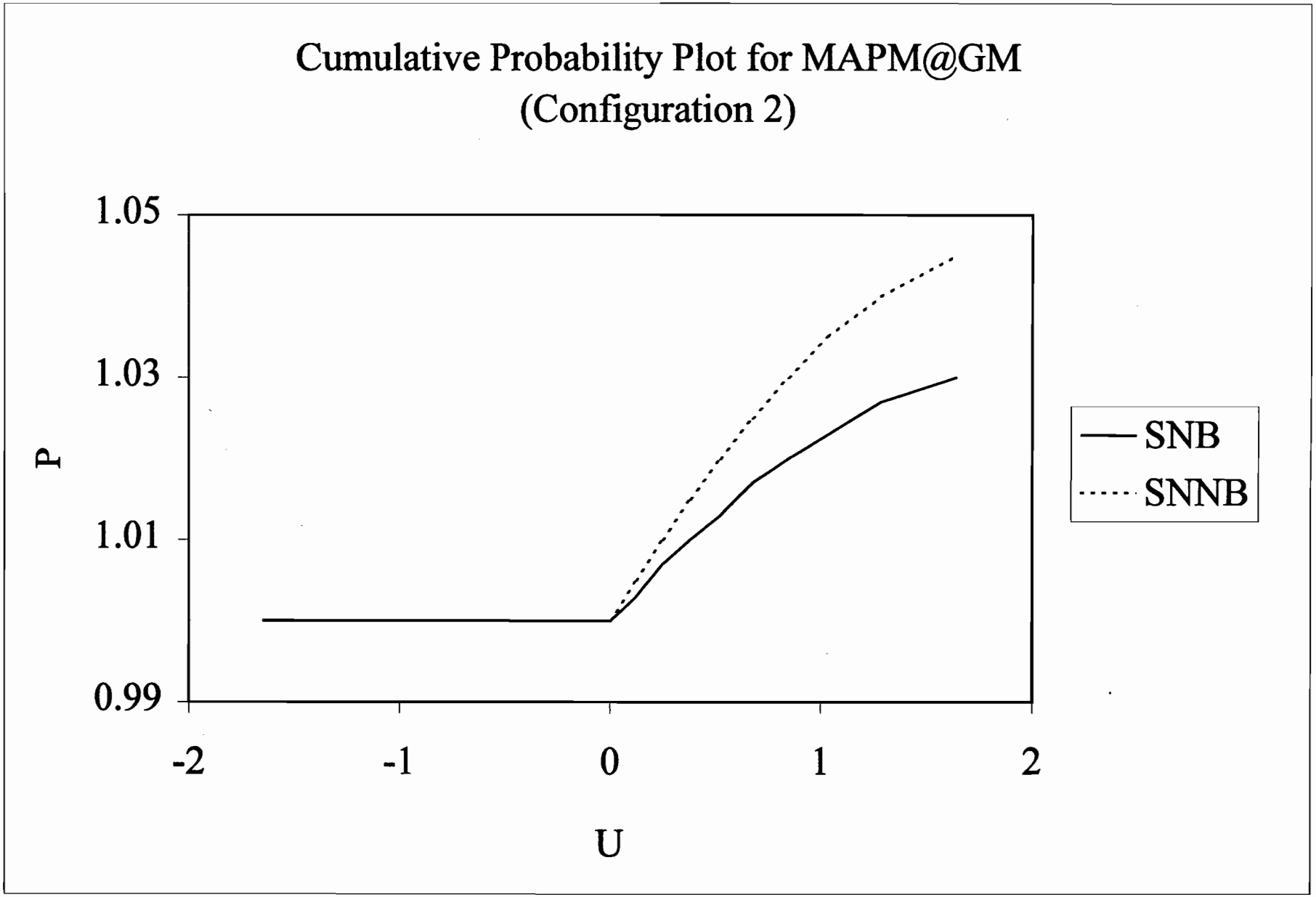
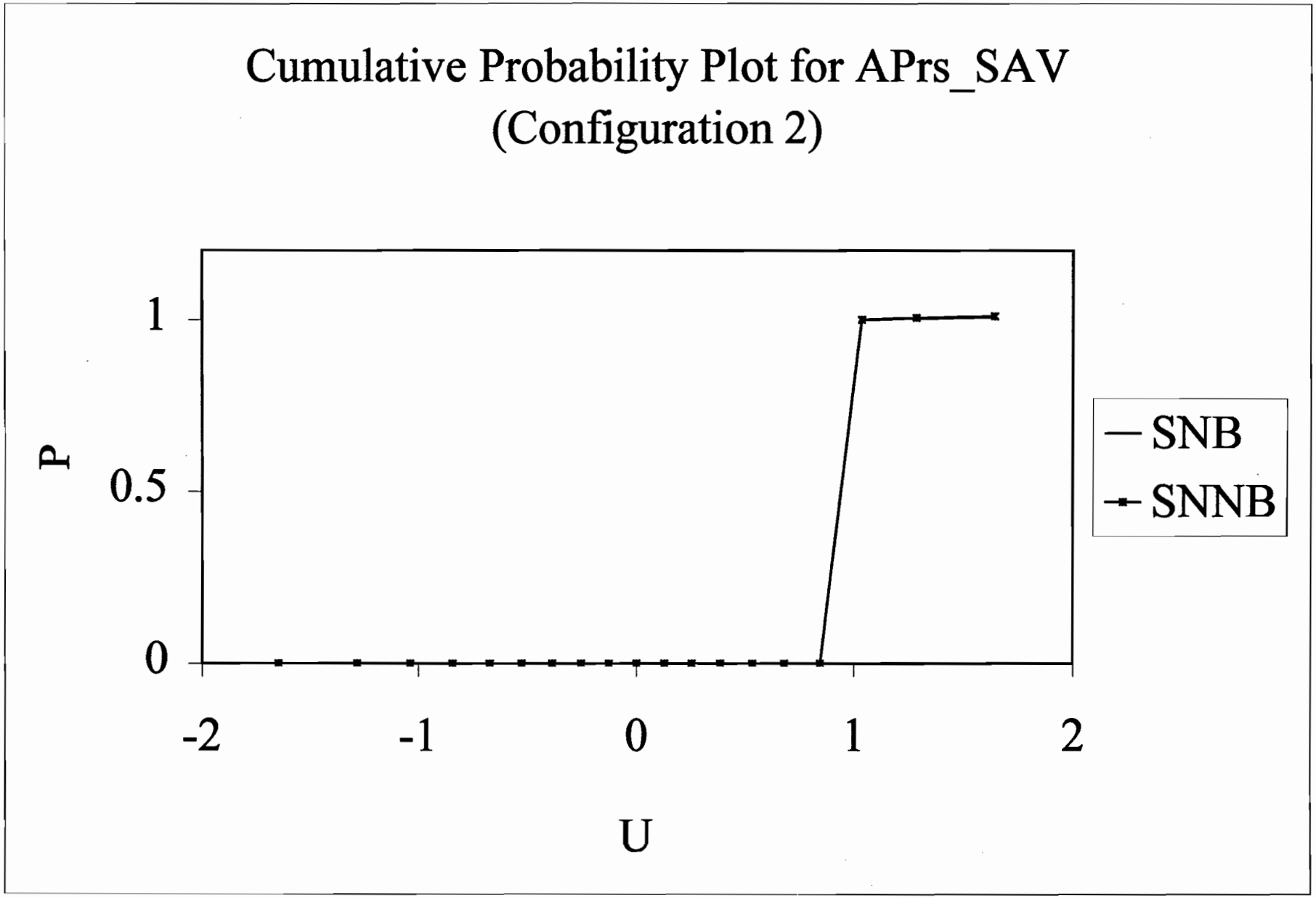
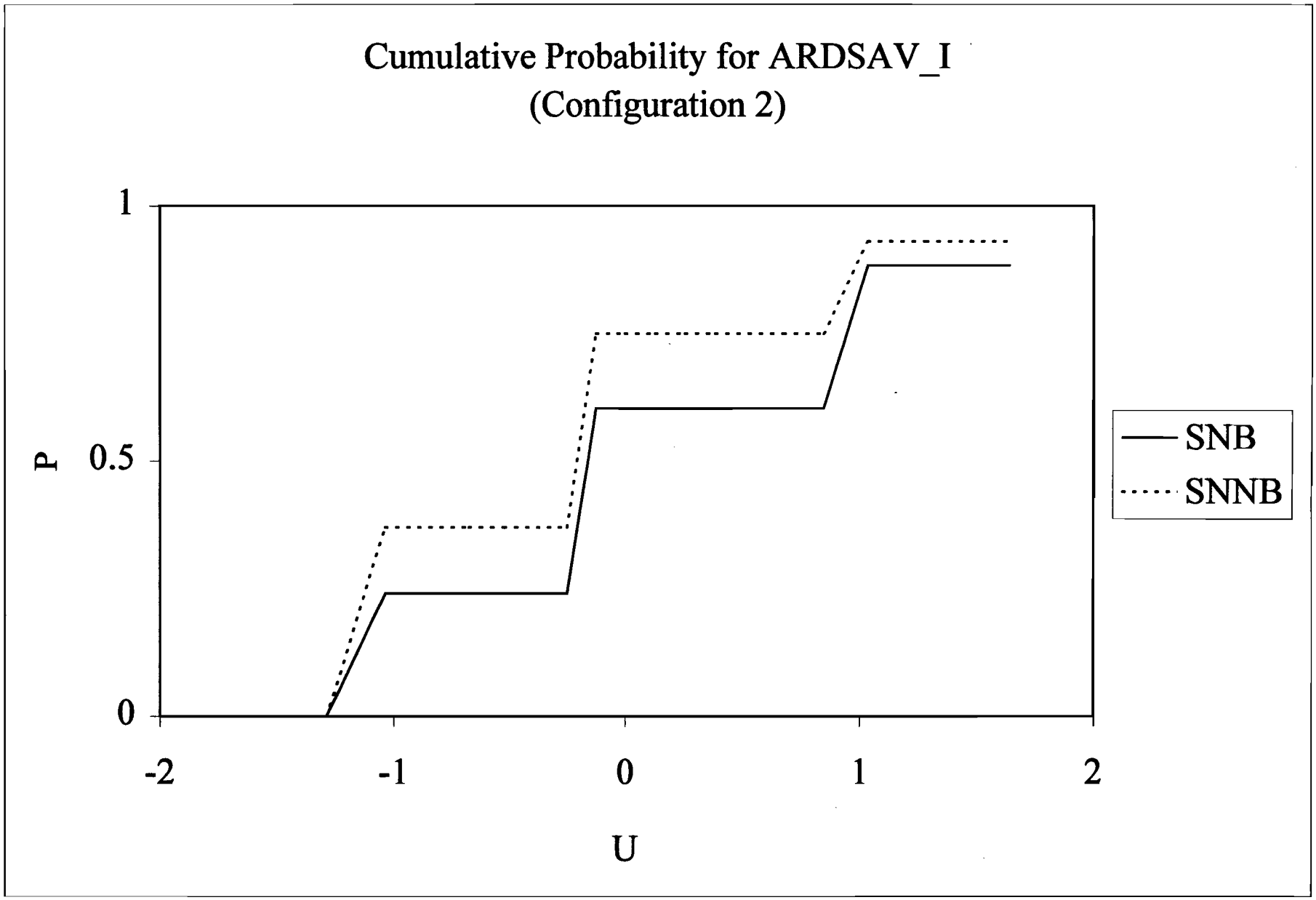
P
-2
-1
0
1
2
U
SNB
SNNB

Cumulative Probability Plot for WPRRG@20 (Configuration 2)




Cumulative Probability Plot for MAPM@GM
(Configuration 2)
1.05
1.03
1.01
0.99
P
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for APrs_SAV
(Configuration 2)
P
1
0.5
0
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability for ARDSAV_I
(Configuration 2)
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P
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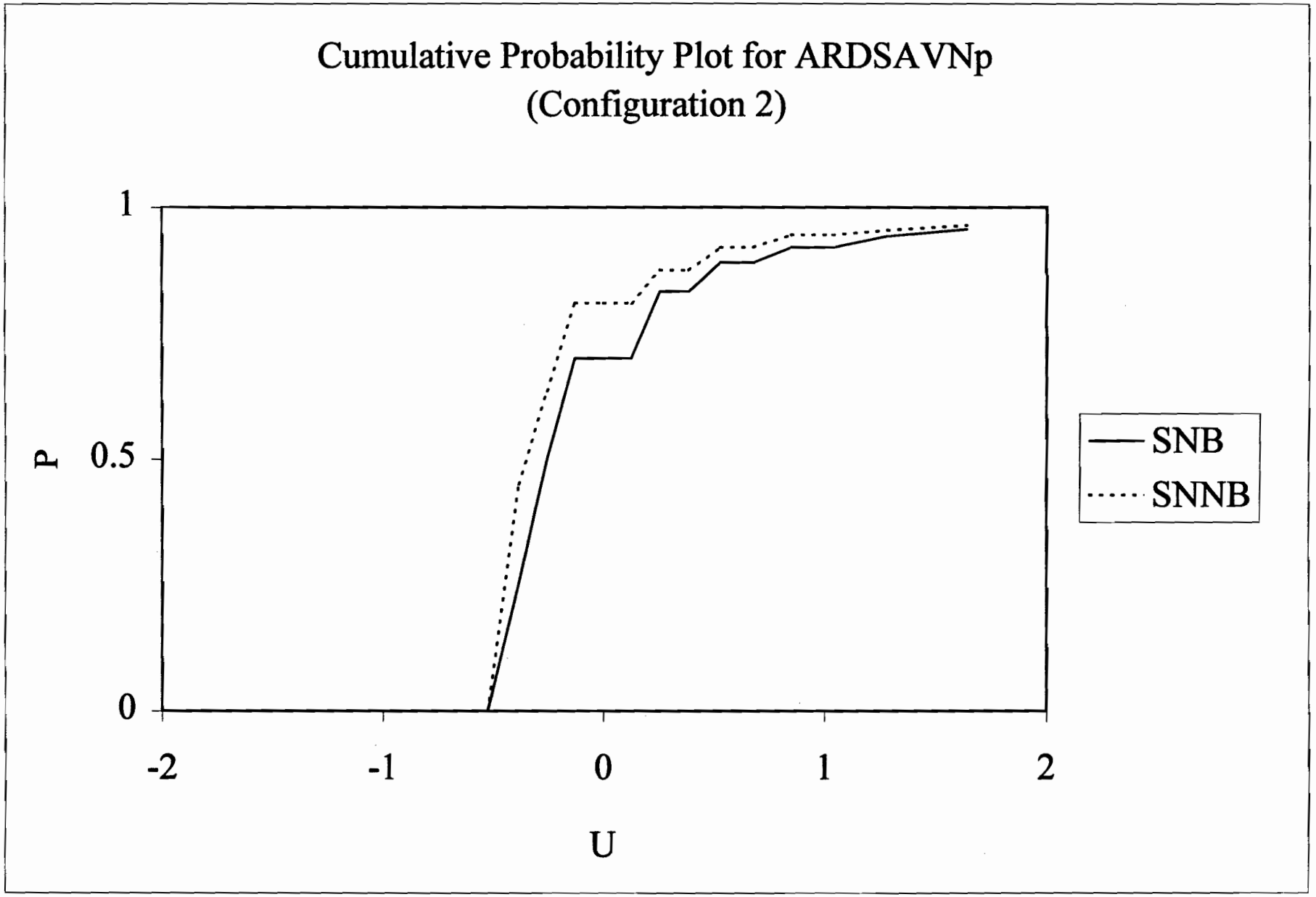
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for ARDSAVNp
(Configuration 2)
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0.5
0
P
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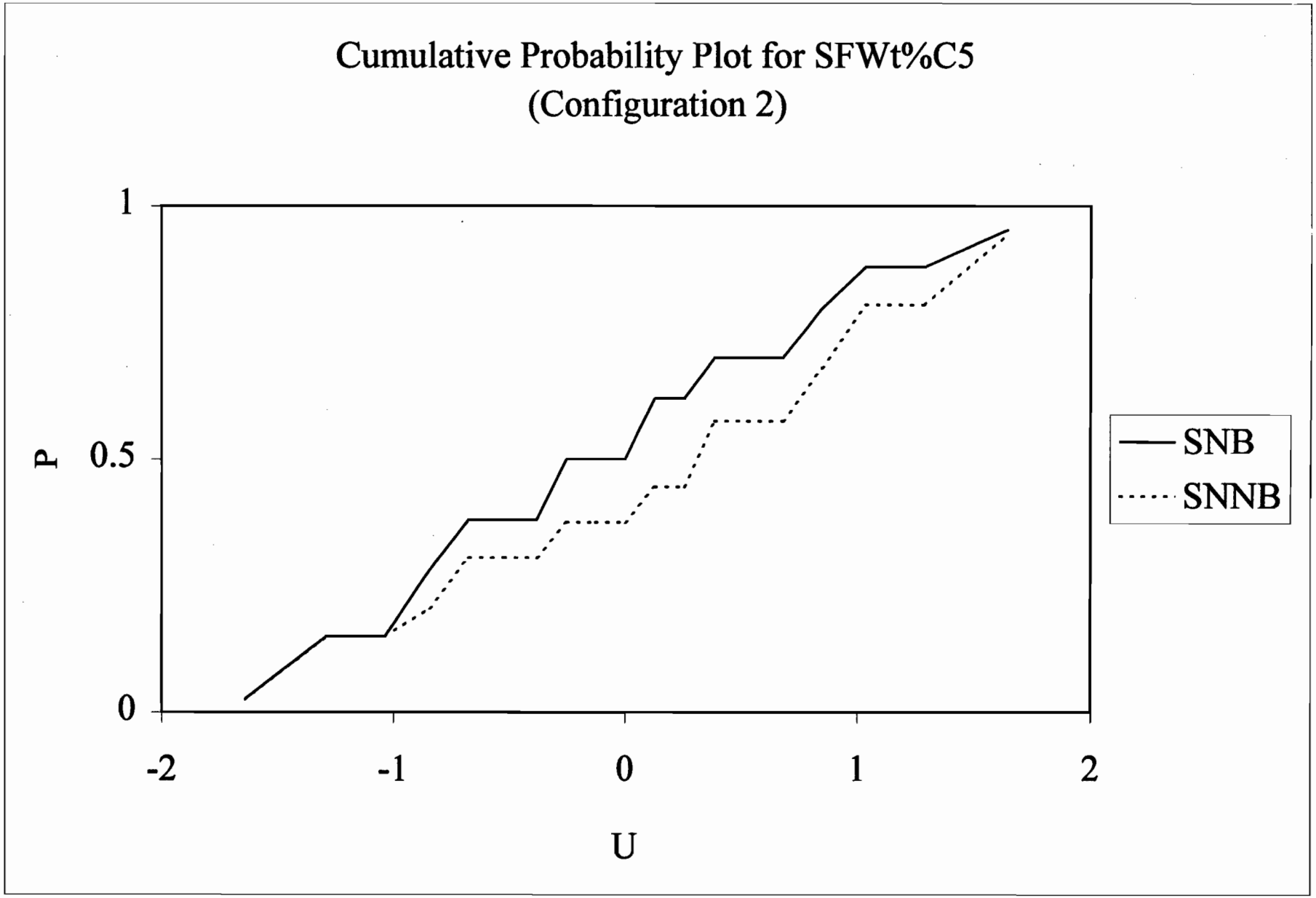
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for SFWt%C5
(Configuration 2)
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P
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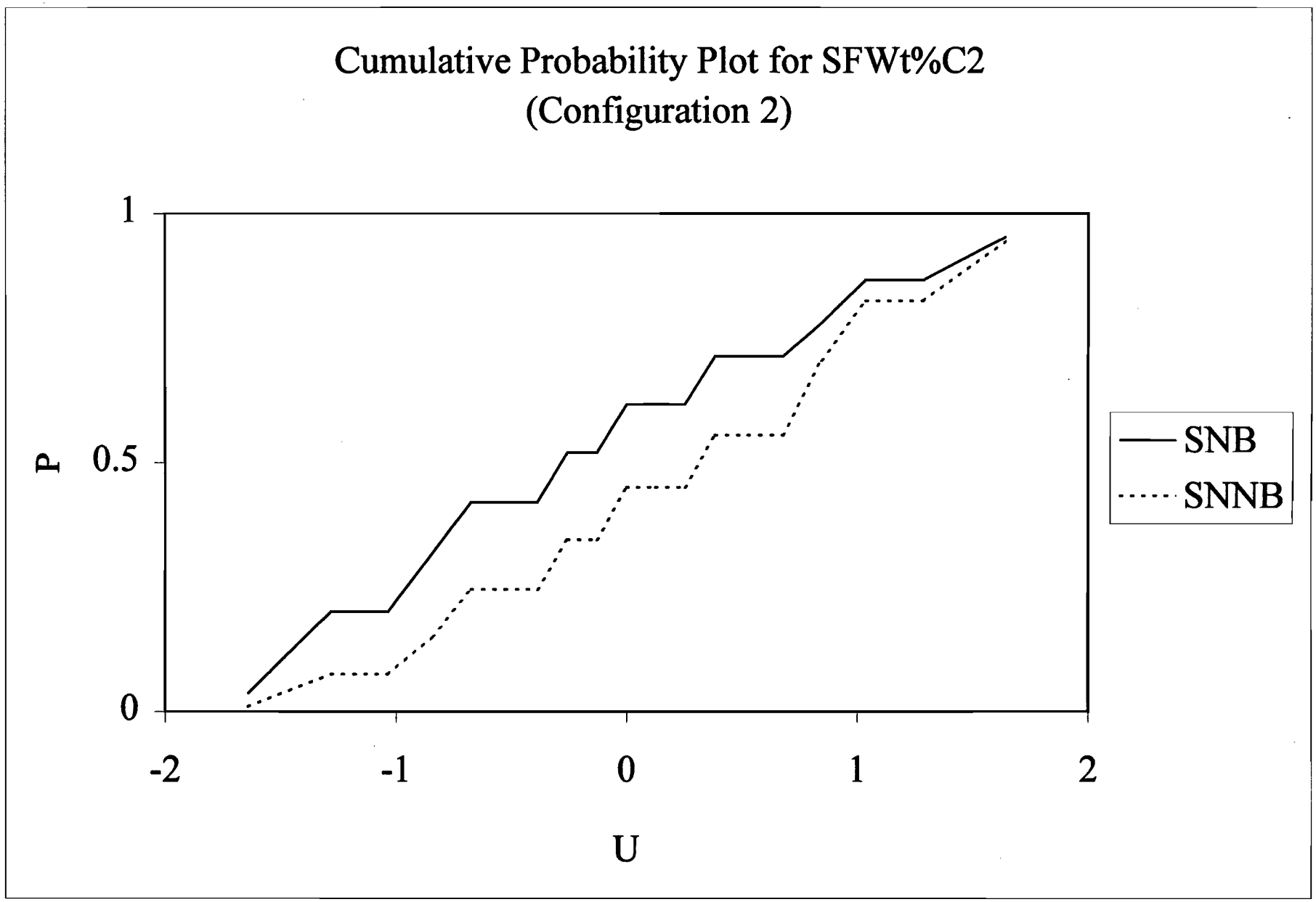
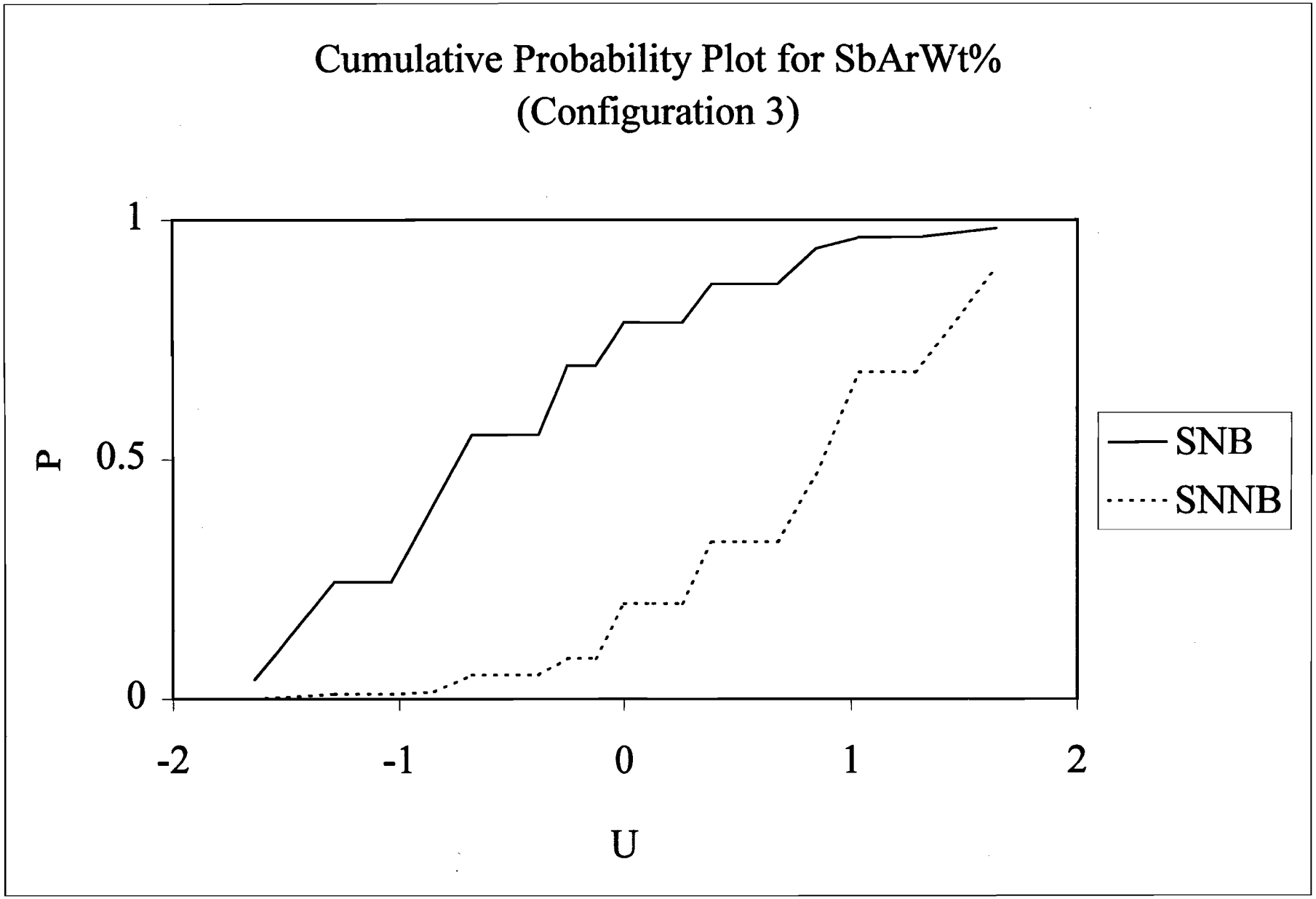
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for SFWt%C2
(Configuration 2)
1
0.5
0
P
-2
-1
0
1
2
U
SNB
SNNB

APPENDIX G


Cumulative Probability Plot for SbArWt%
(Configuration 3)
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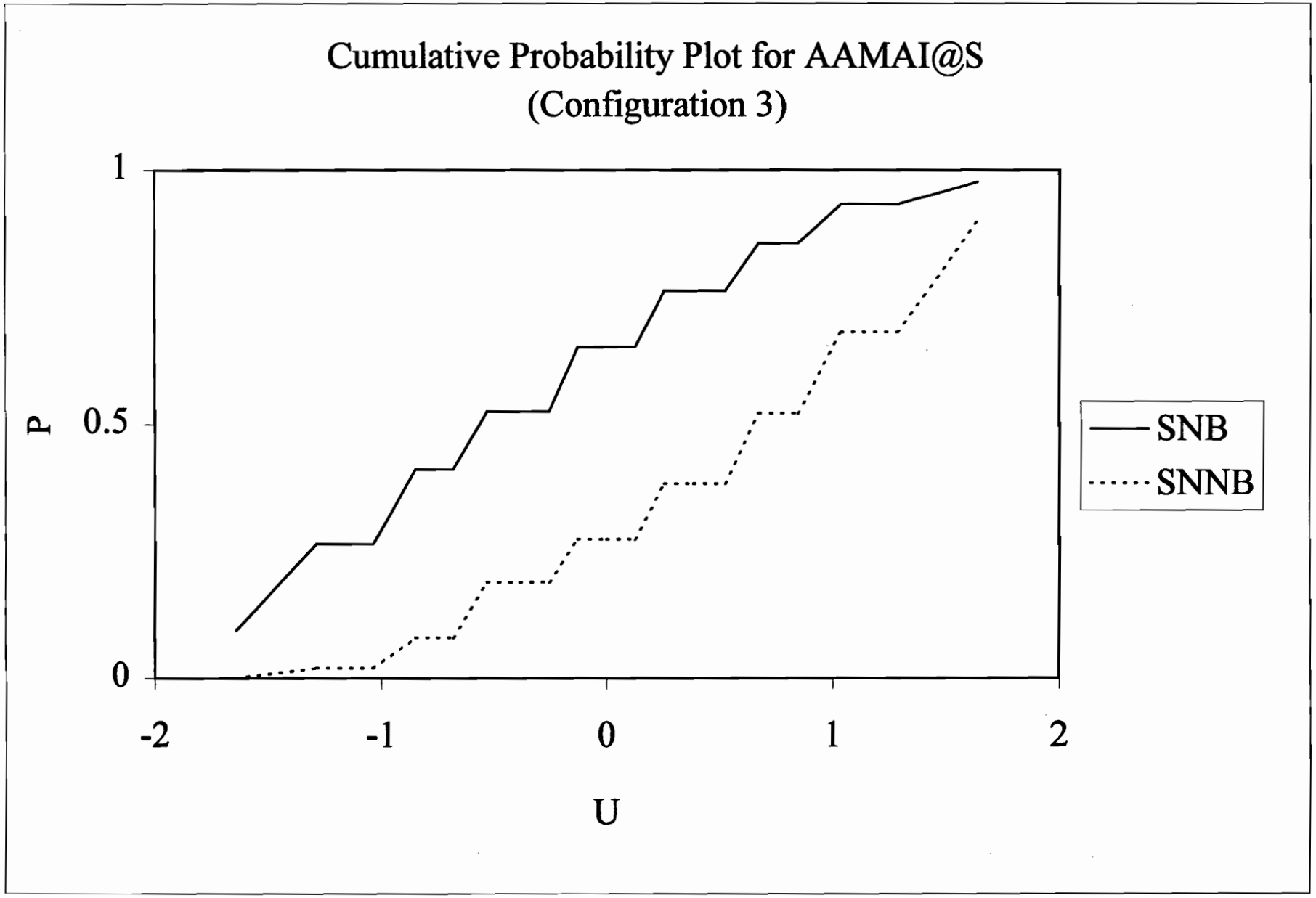
0.5
0
P
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for AAMAI@S
(Configuration 3)
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P
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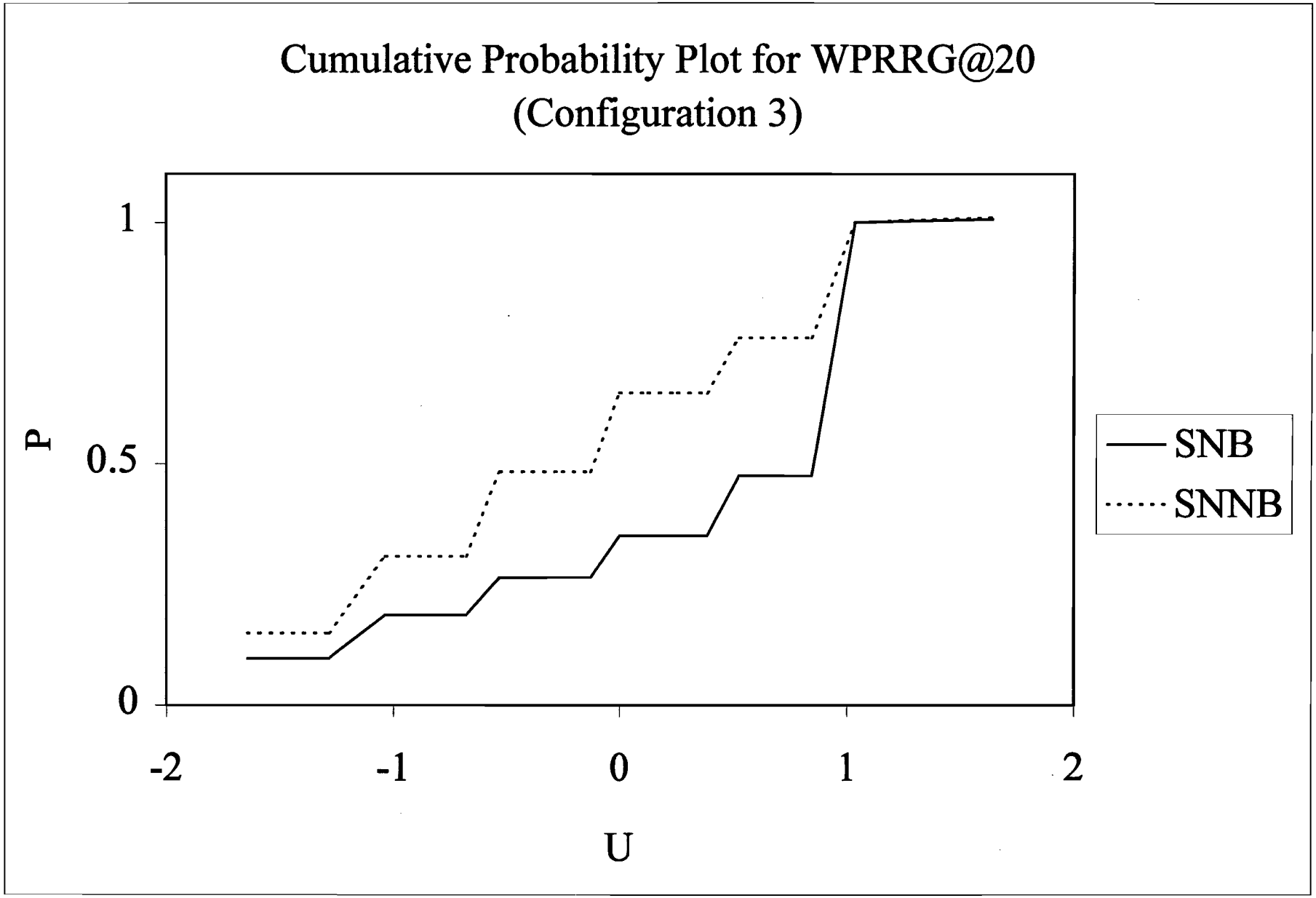
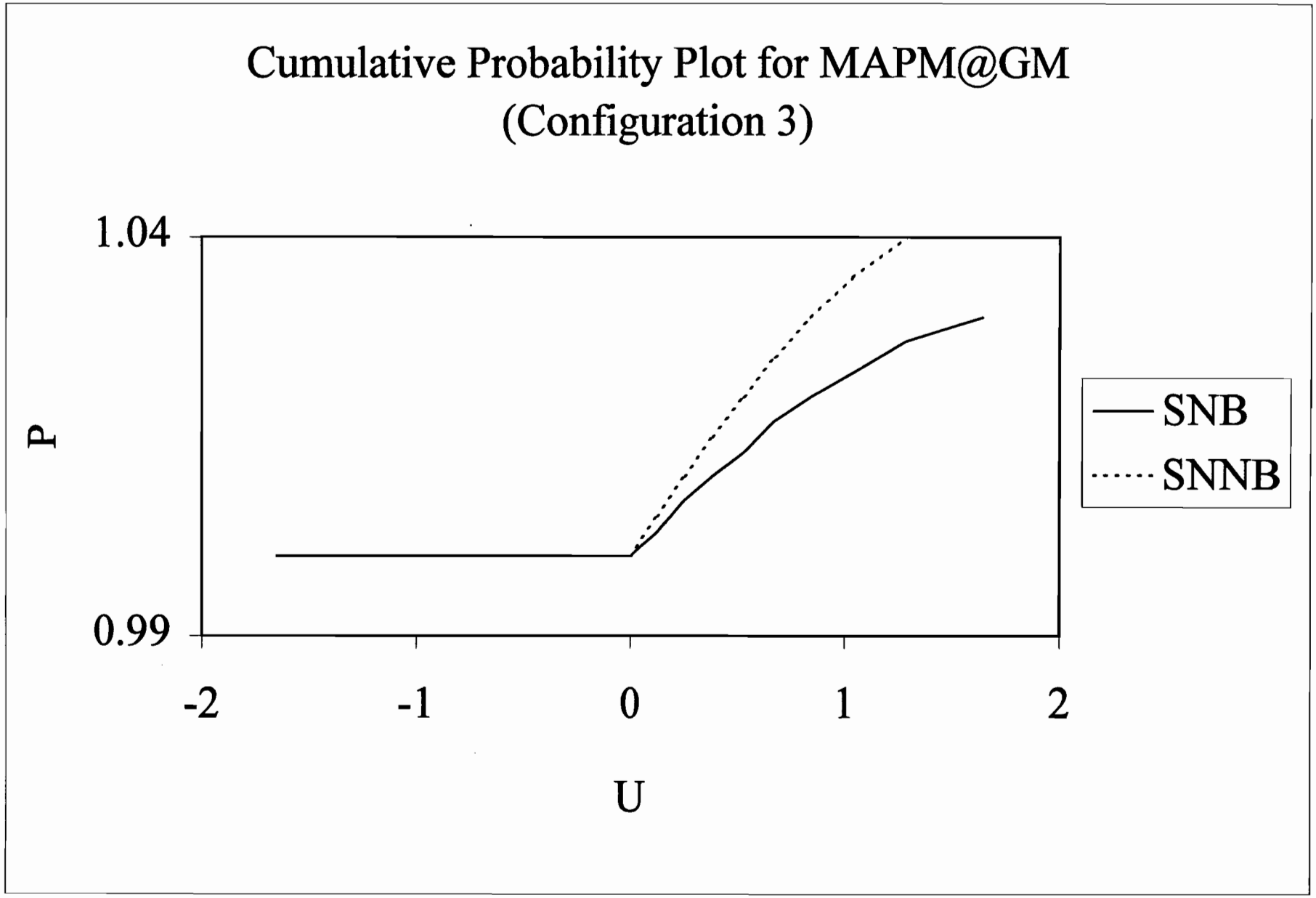
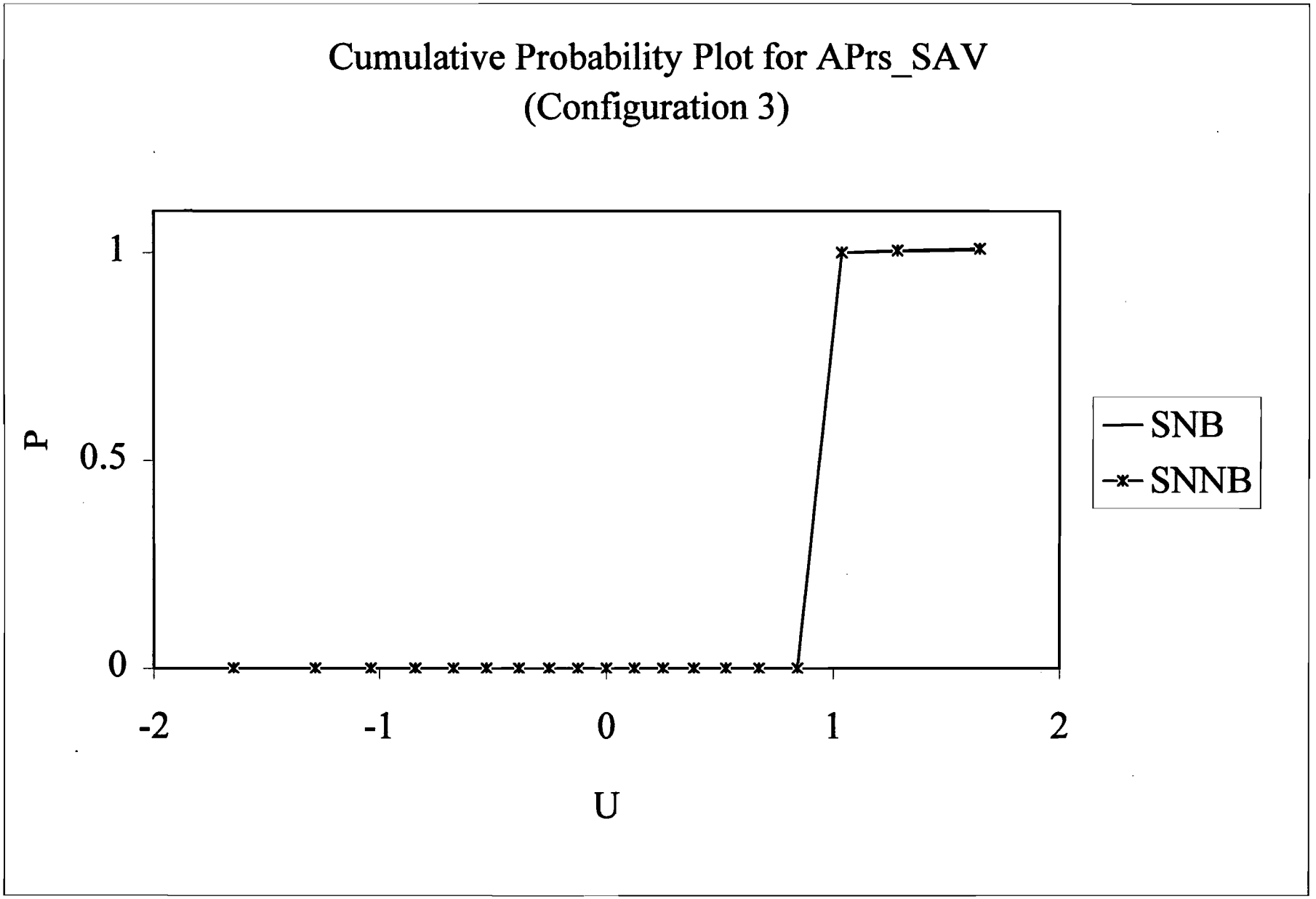
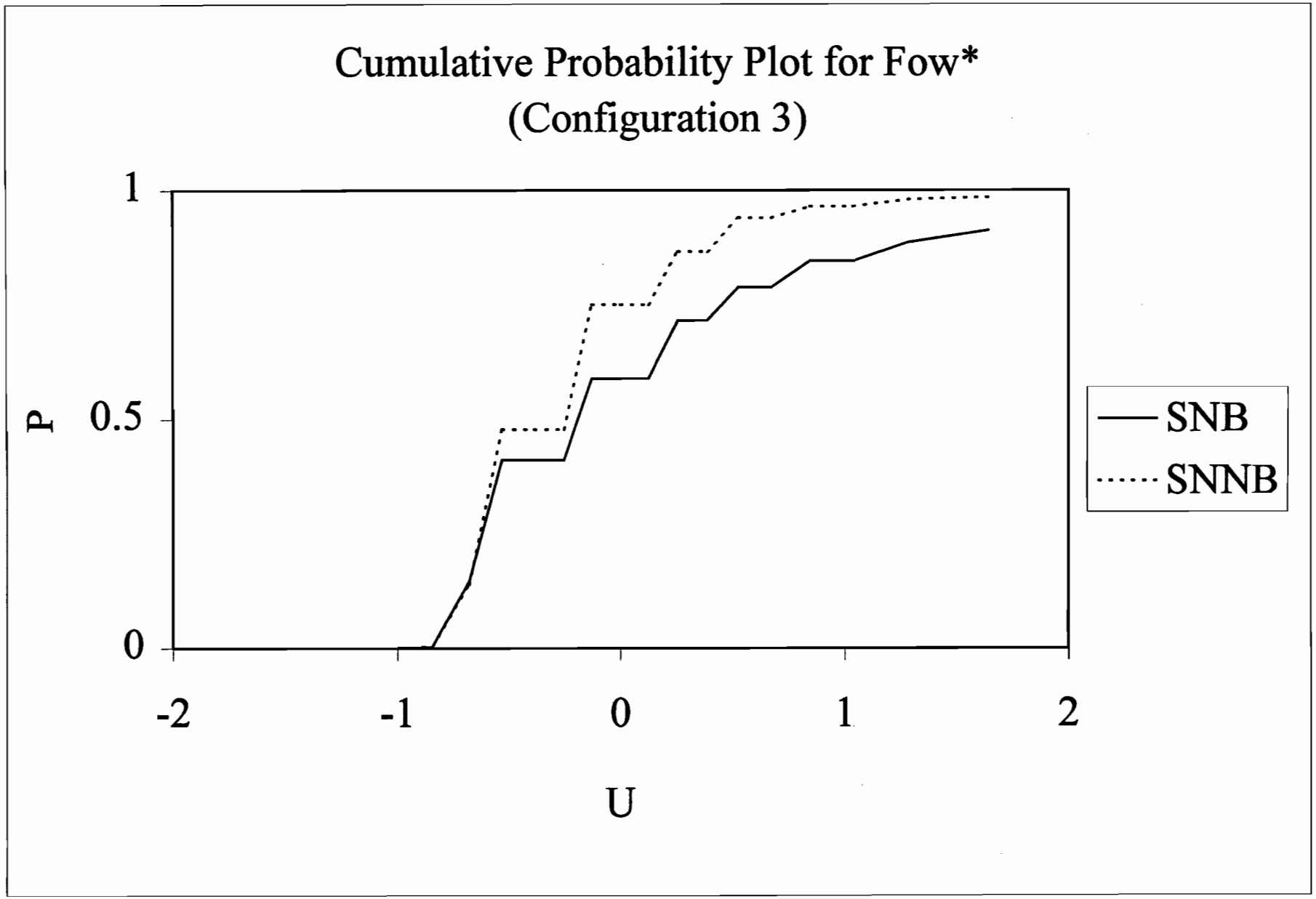
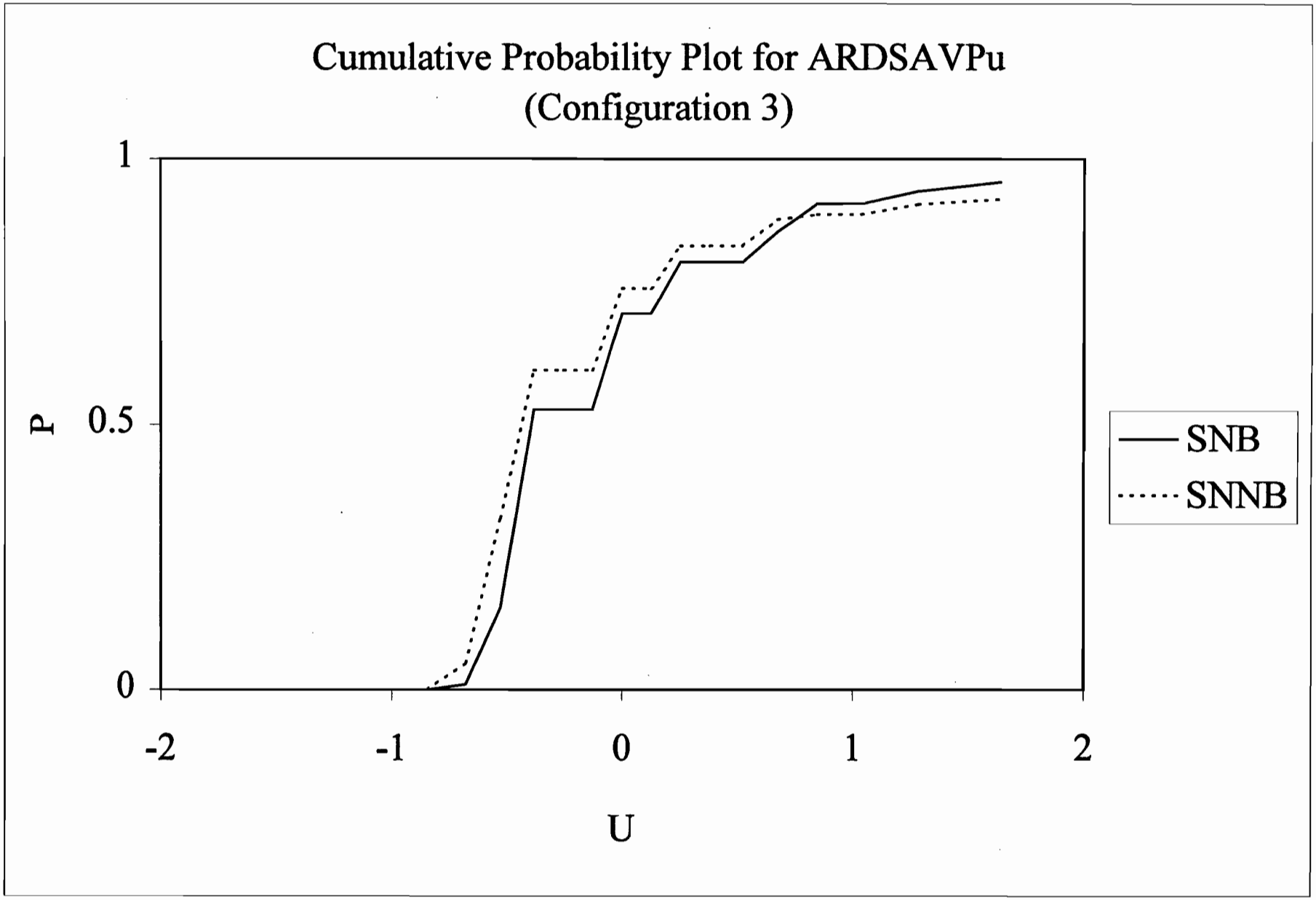
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for WPRRG@20
(Configuration 3)
P
1
0.5
0
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for MAPM@GM
(Configuration 3)
1.04
0.99
P
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for APrs_SAV
(Configuration 3)
P
1
0.5
0
-2
-1
0
1
2
U
SNB
SNNB


Cumulative Probability Plot for Fow*
(Configuration 3)
1
0.5
0
P
-2
-1
0
1
2
U
SNB
SNNB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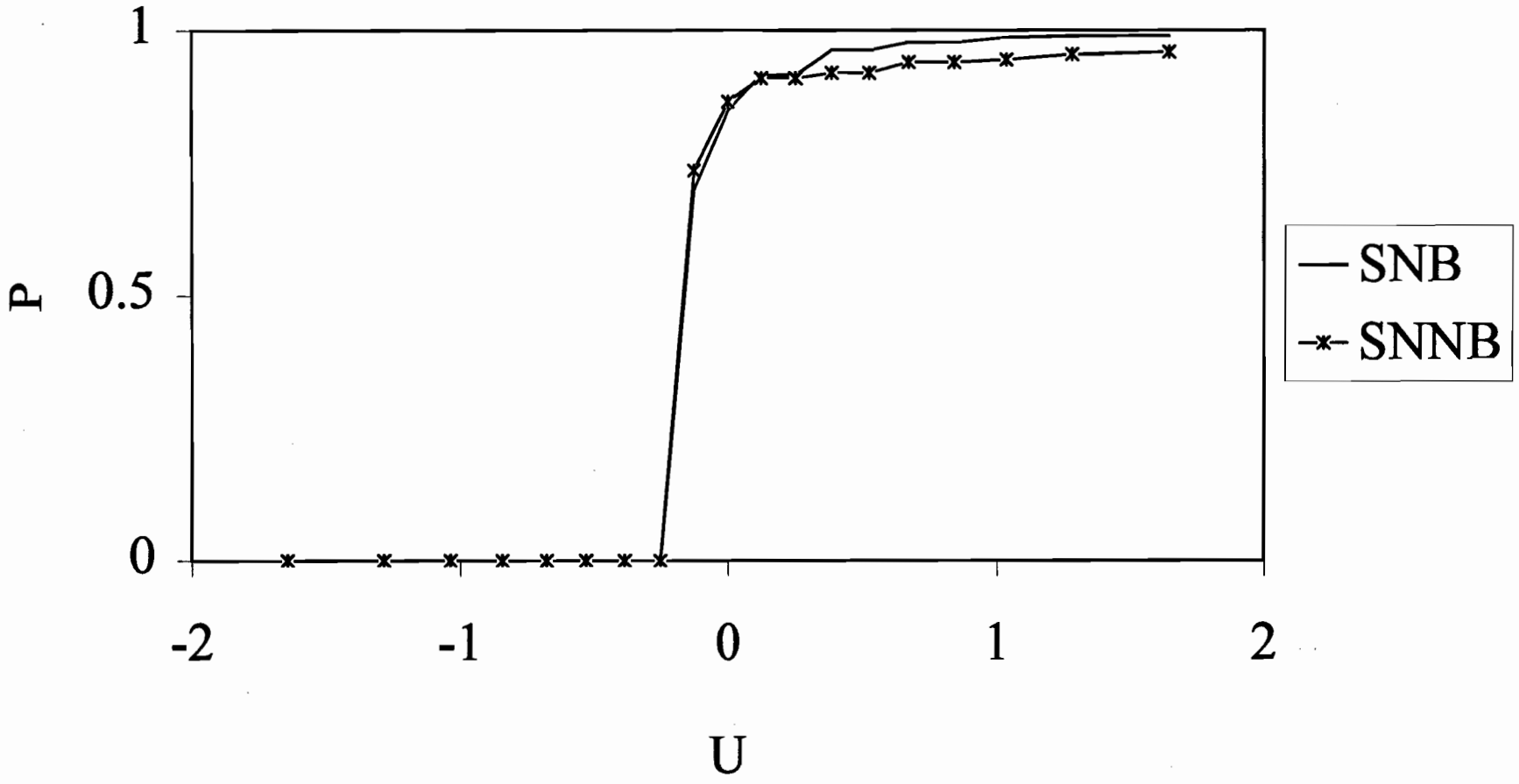

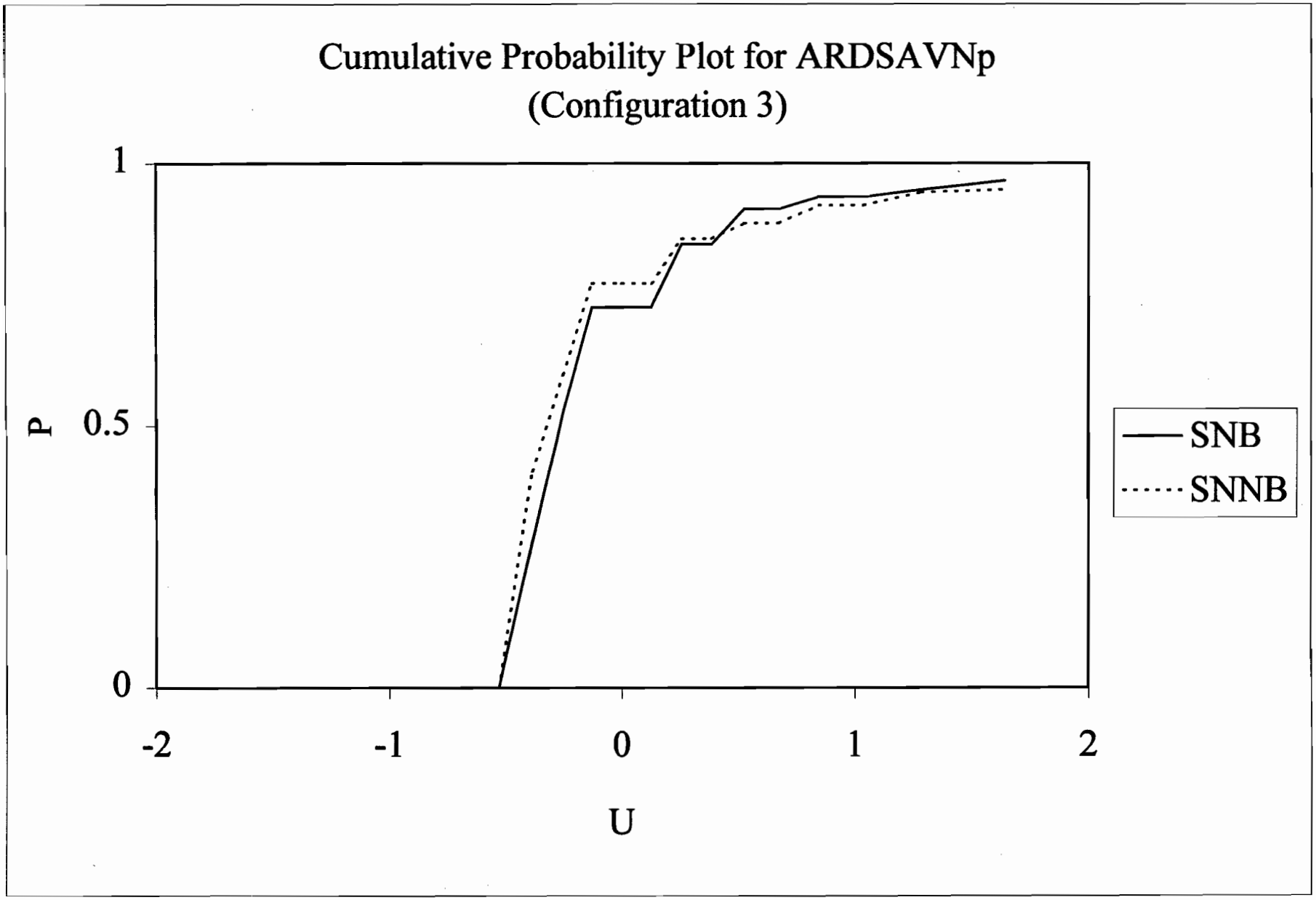
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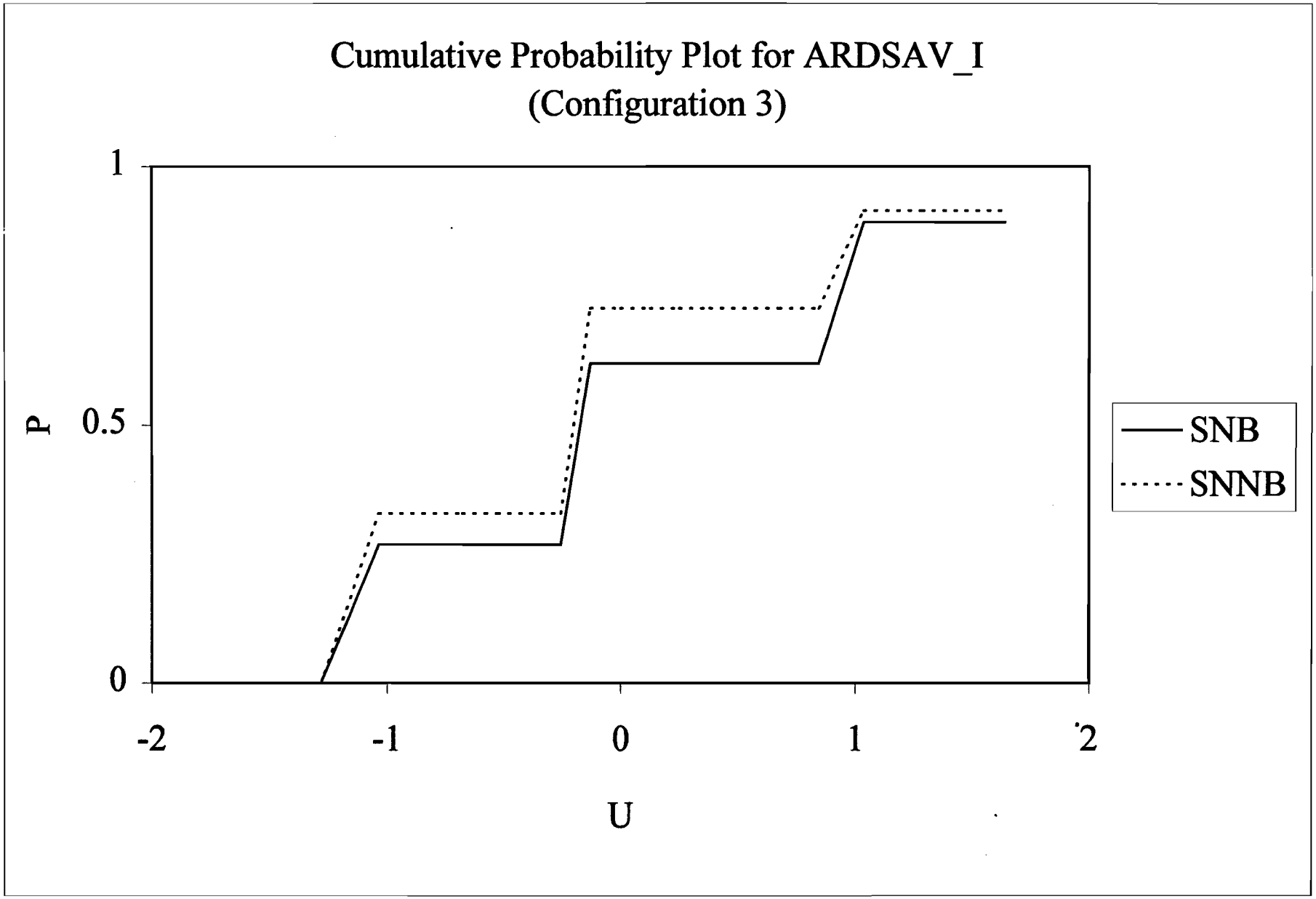
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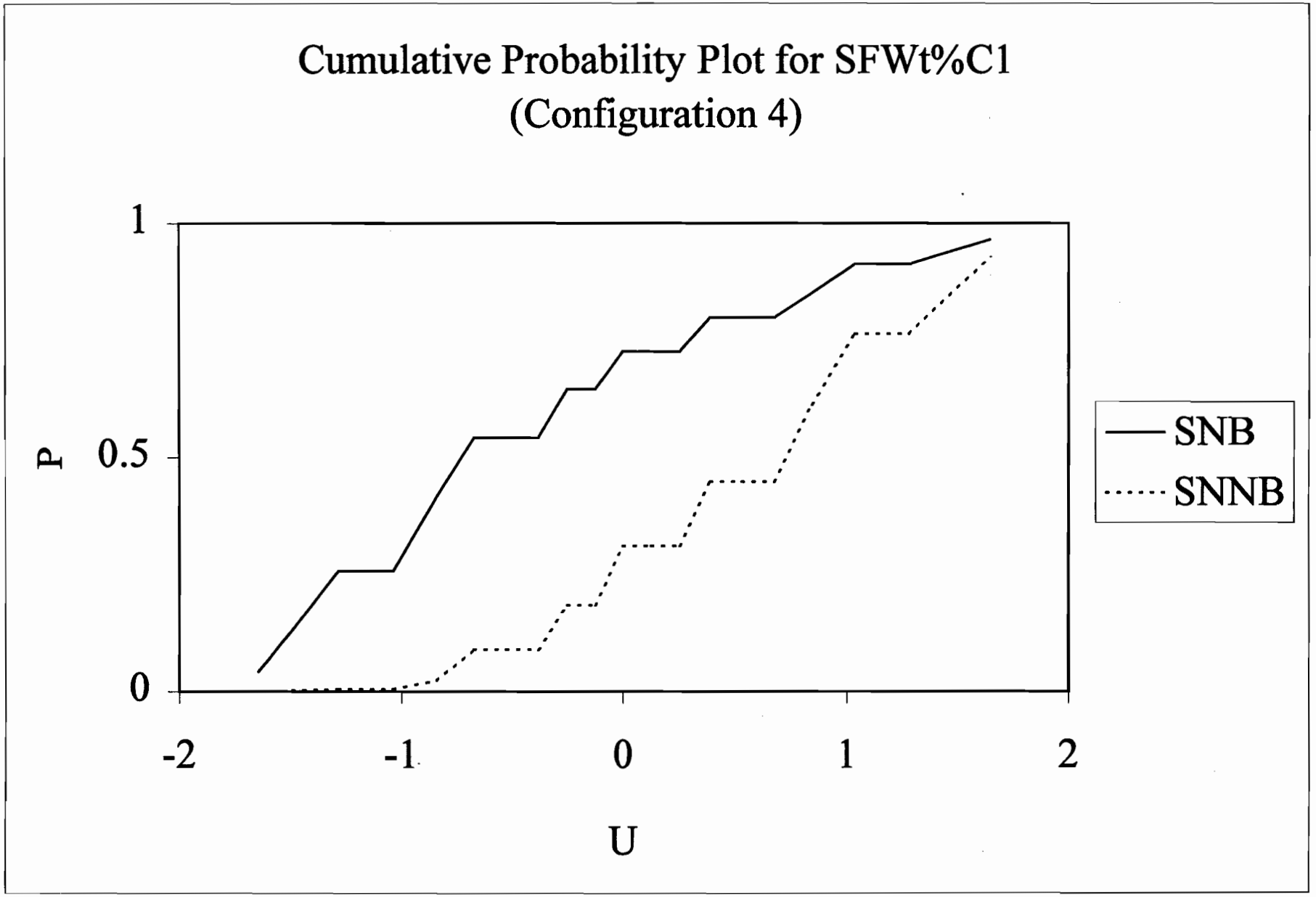
APPENDIX H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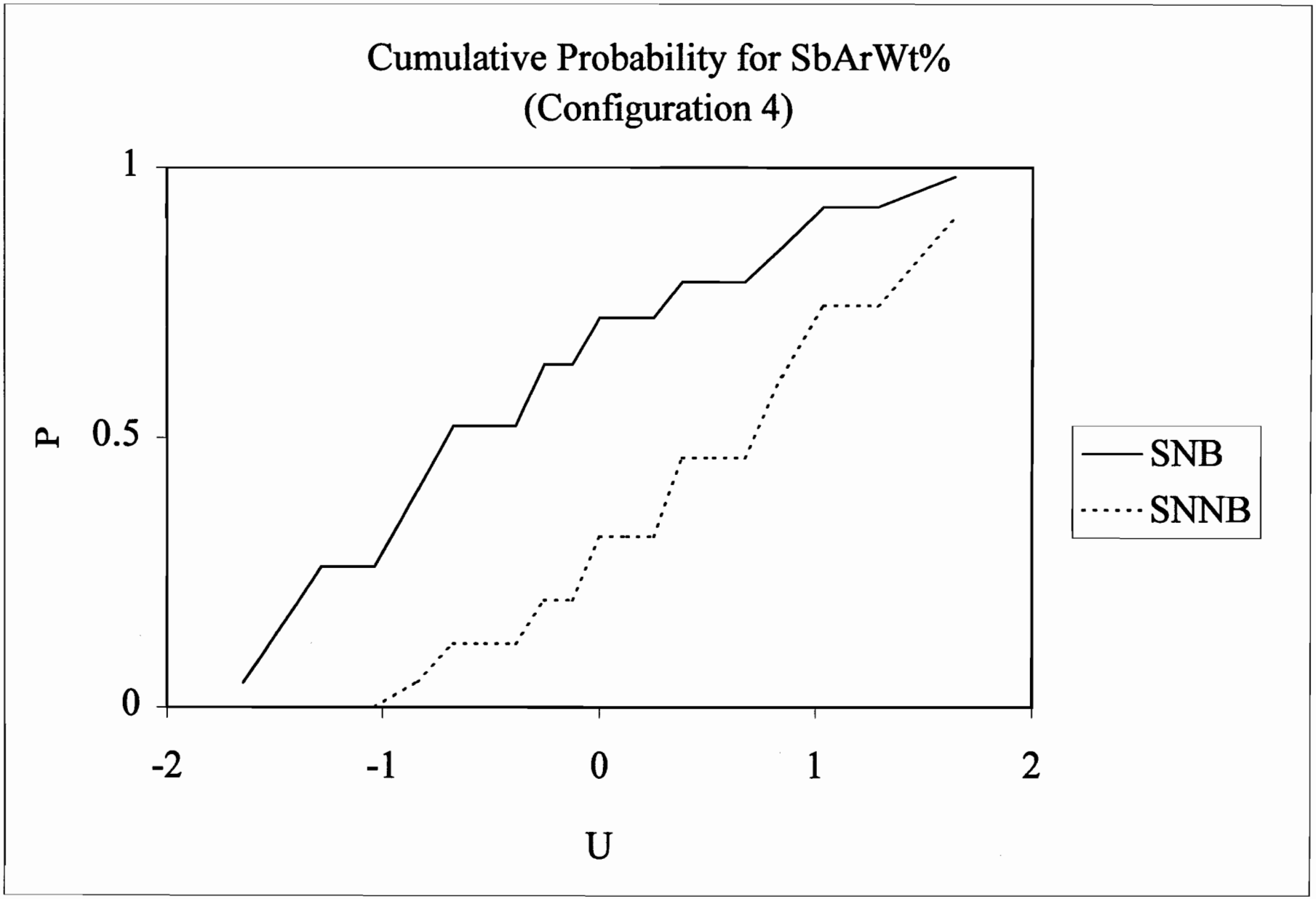
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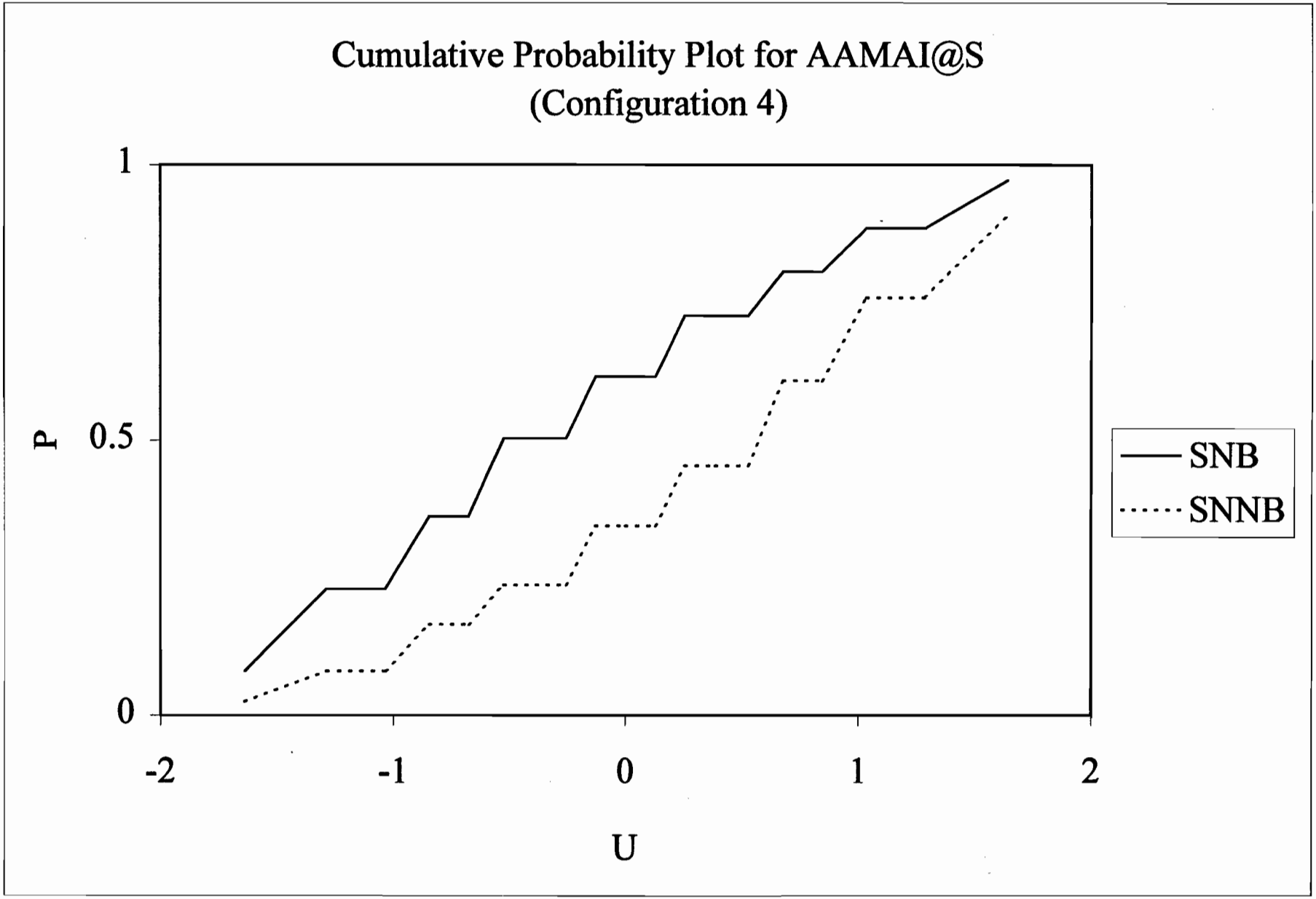
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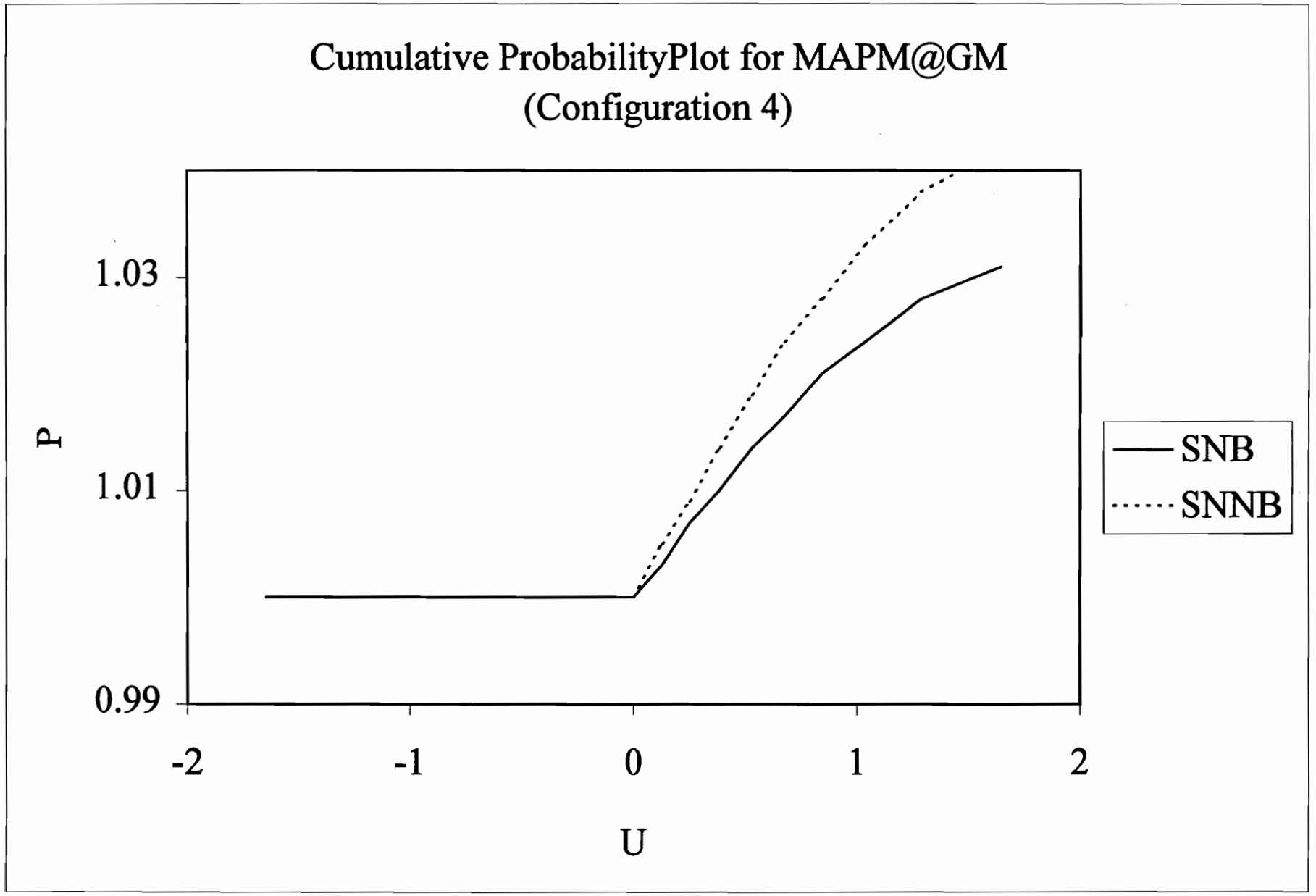
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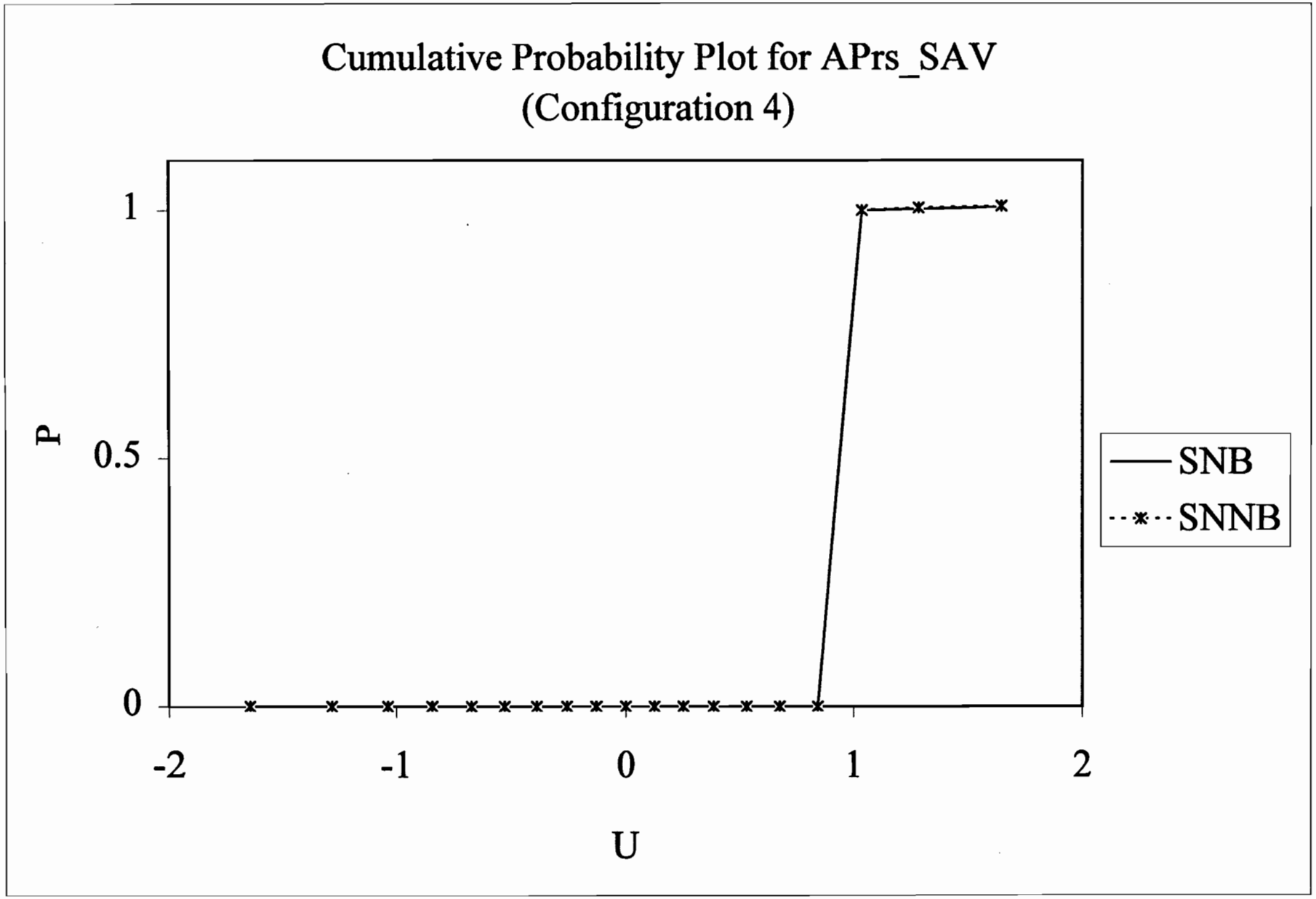
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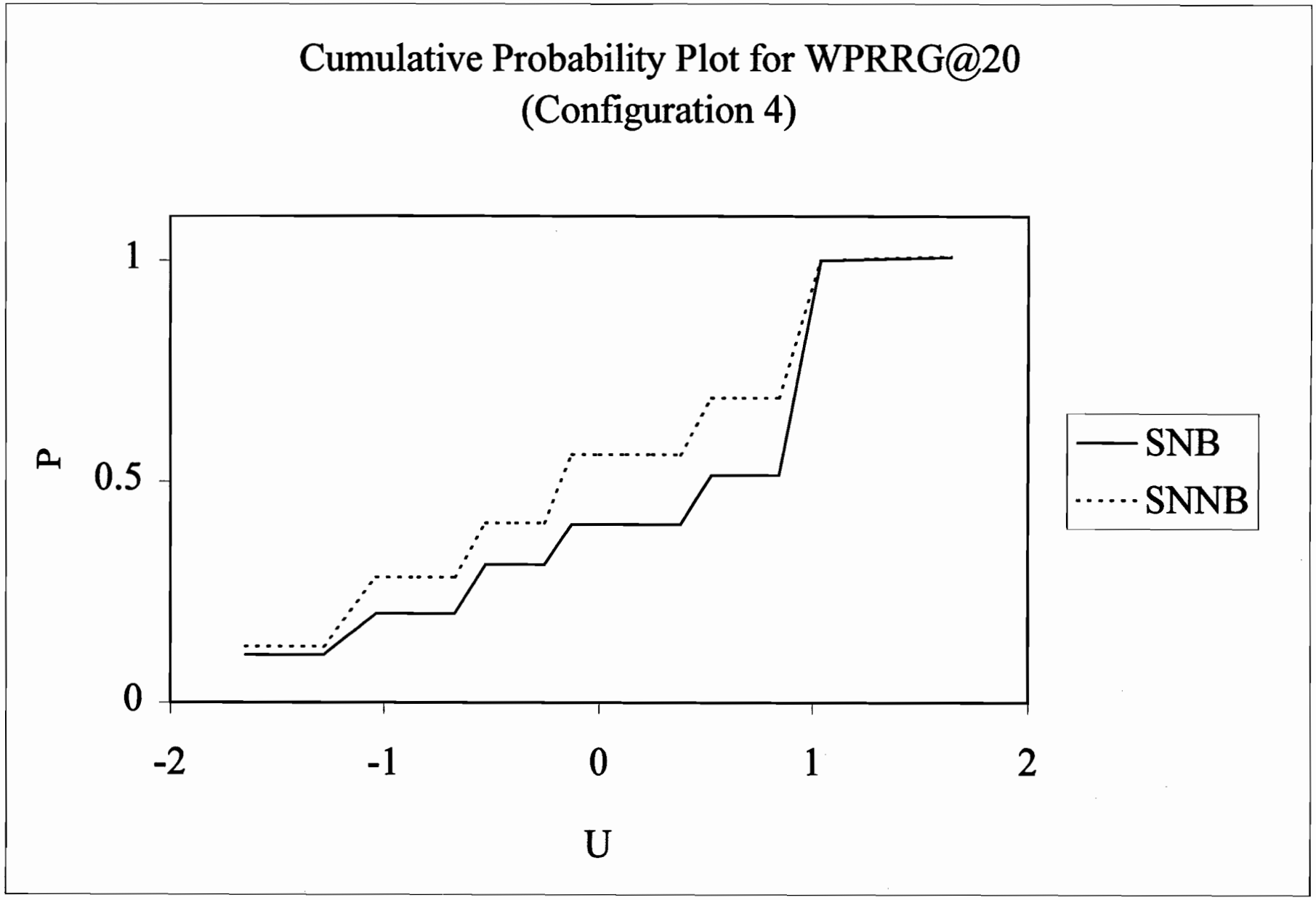
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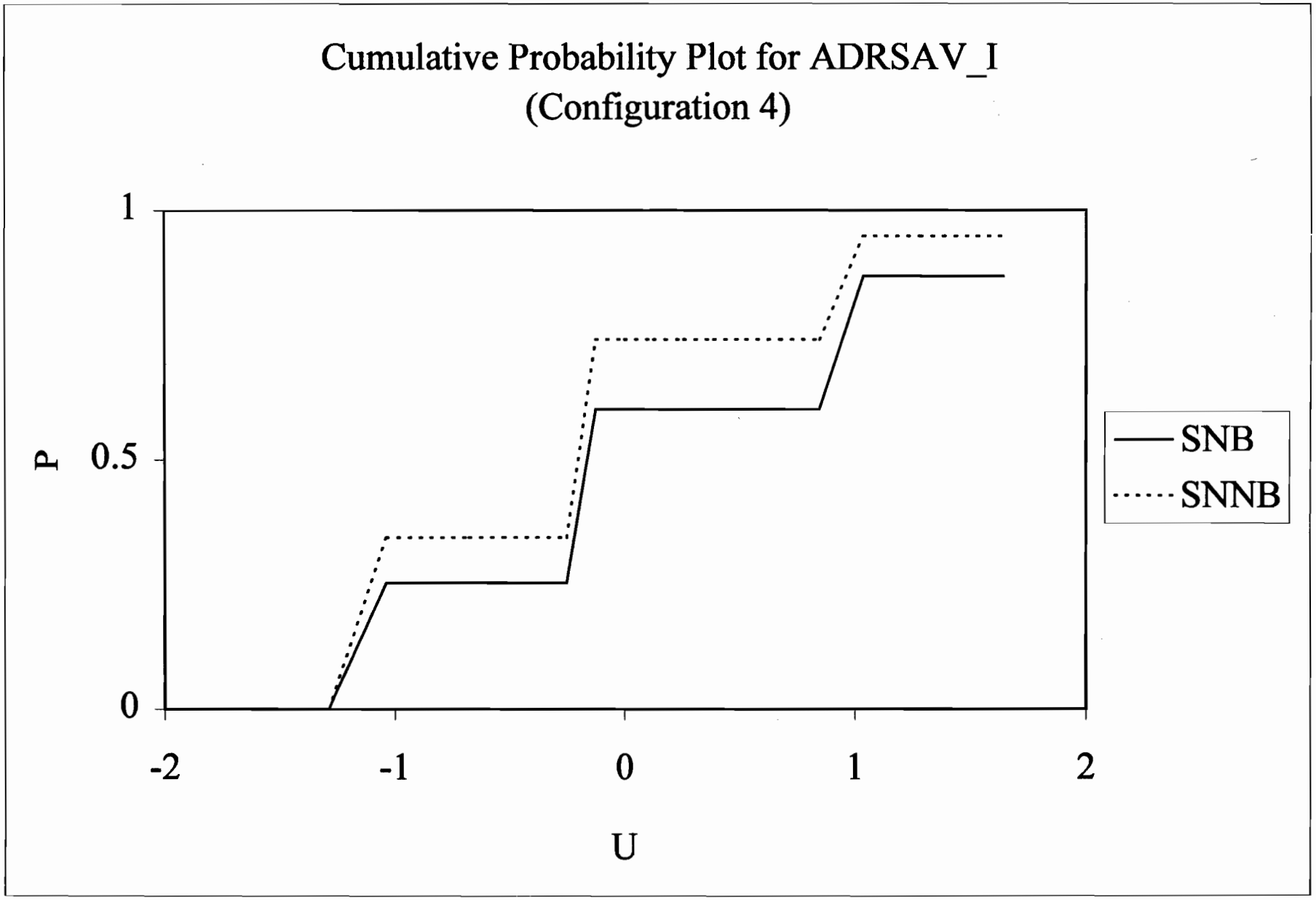
Cumulative Probability Plot for ADRSAV_I
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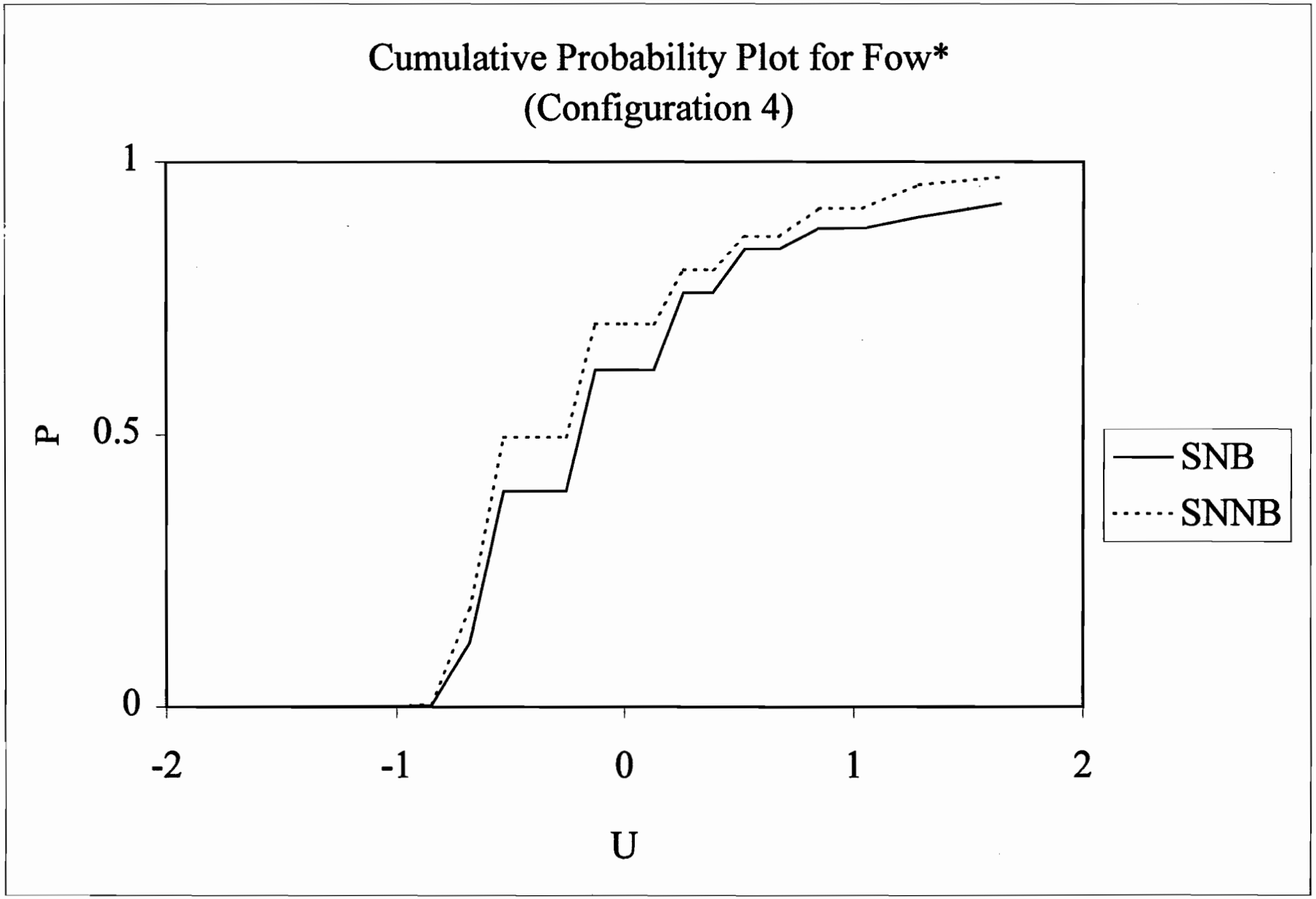
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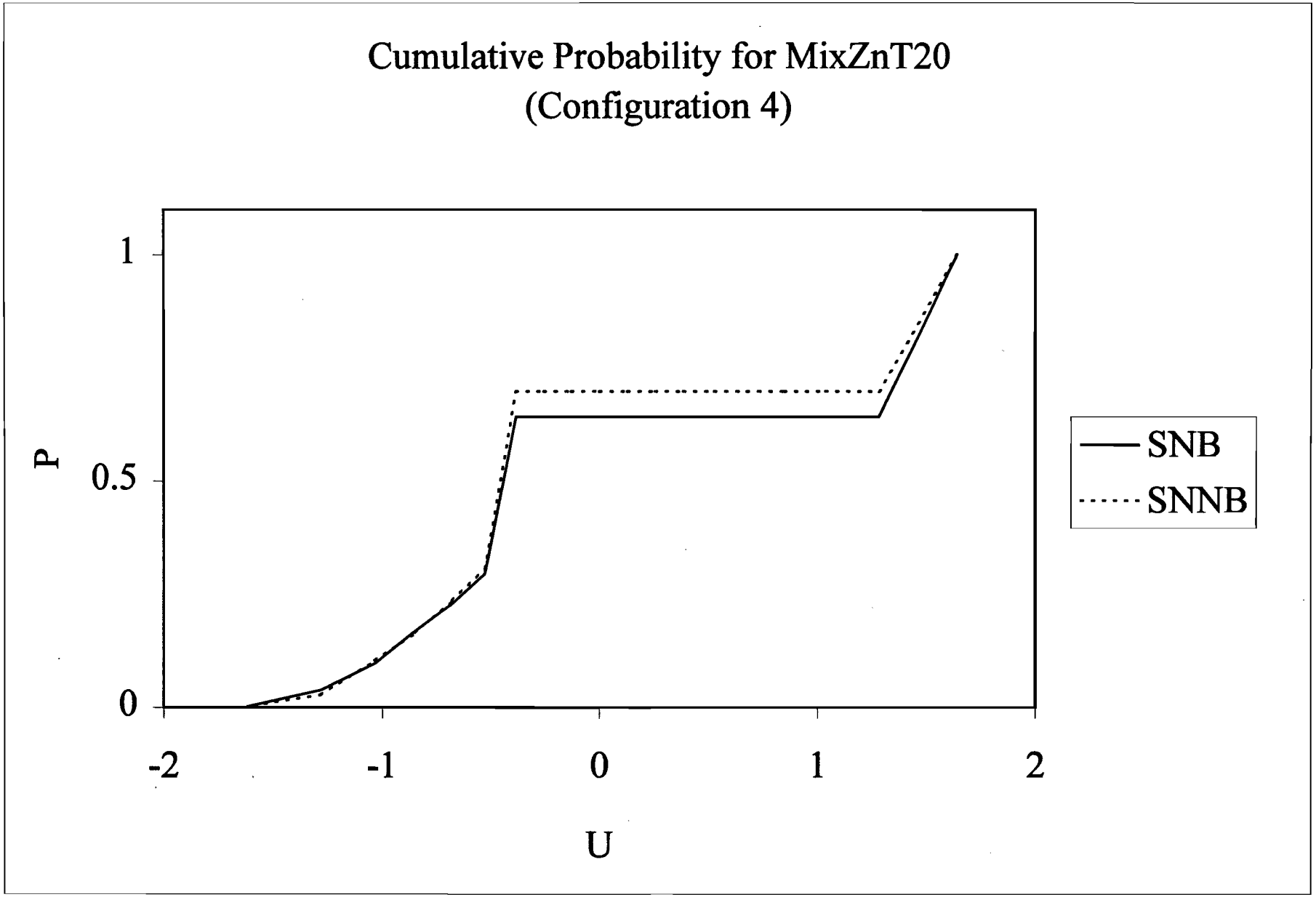
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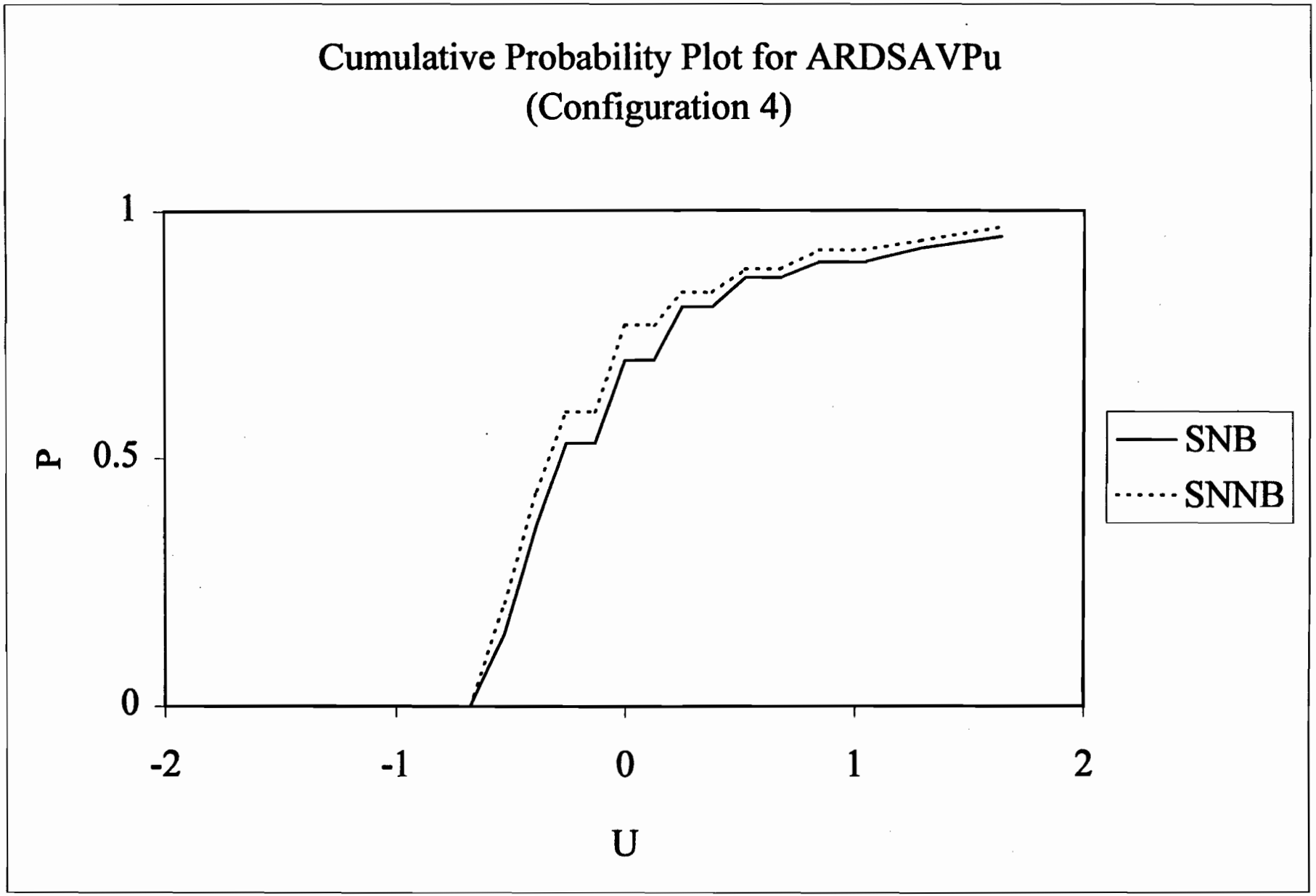
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DEPARTMENT OF ENVIRONMENTAL SCIENCES

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5 July, 1999

Andy C. Campbell
Advisory Committee on Nuclear Waste
U.S. Nuclear Regulatory Commission
WASHINGTON, DC, 20555

Dear Andy,

Enclosed is a copy of a paper that appeared in the ***Journal of Environmental Management*** that covers the idea that I had for another examination of Monte-Carlo results from the TPA-3 code. (I also enclose a few other reprints that may be helpful in visualizing how the analysis might go.) Basically, the idea is similar to that covered in Dick Codell's "t-test" results. What I envision is an analysis of the Monte-Carlo results in the context of a dose standard, rather than just a simple statistical investigation. Because the results at 10,000 years do not show violations of any reasonable standard, I would suggest that we use 50,000 years for illustrative purposes. This approach might be OK anyway in the context of a conservative regulatory approach. I list below a possible way for us to proceed.

(1) Get results from Monte-Carlo runs. If we can get the 4,000 runs used by Norm and Budhi, that would be great. If so, we can do the analysis below for four separate 1,000-realization runs and look at the robustness to sample size. If not, then we could just use Dick Codell's 1000 realizations and worry about robustness later.
(2) Choose a criterion (or criteria) for an acceptable behavior. I suggest a dose of less than 5 mrem at 50,000 years. (The argument might be that if there are aspects of the model that lead to this level of dose at 50,000 years, then these aspects can be viewed as critical uncertainties for meeting the standard as well.)
(3) Write a code to go through the realizations and determine whether the run is acceptable or unacceptable; write the parameters for behaviors in one file and for non-behaviors in a second file.
(4) Analyze the differences between the two bins of parameters. (I have a FORTRAN code for the analysis that we can use as is or can modify as we see fit.) The analysis looks at covariances as well as simple univariate separations.

Let me know if you think this idea is worth pursuing. As long as we don't have to exercise the TPA code ourselves, I think the effort would not be too burdensome.

Best regards,

Journal of Environmental Management (1981) **12**, 7–18

An Approach to the Preliminary Analysis of Environmental Systems

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Received 2 *October* 1979

In the preliminary analysis of environmental problems, mathematical modelling studies can sometimes aid in hypothesis development and in the integration of preliminary data. Circumstances usually require models used in this way to be simulation models closely based on traditional scientific descriptions of component processes. As a result, such models contain many ill-defined parameters, a fact which severely limits the reliance that can be placed on the outcome of any single simulation. In an attempt to overcome this difficulty, it has been proposed that parameters be assigned statistical distributions which reflect the degree of parametric uncertainty and that these distributions be used in Monte Carlo simulation analyses. We propose a variation on this theme in which we first stipulate the systems' problem-defining behaviour and define a classification algorithm to be applied to the model's output. This algorithm results in each simulation run being classified as a behaviour, B, or not a behaviour, $\bar{B}$. The parameters leading to the result are stored according to the behavioural outcome. Subsequently, all parameter vectors are subjected to analysis to determine the degree to which the *a priori* distributions separate under the behavioural mapping. This separation, or lack thereof, forms the basis for a generalized sensitivity analysis in which parameters and their related processes important to the simulation of the behaviour are singled out. The procedure has been applied to a eutrophication problem in the Peel–Harvey Inlet of Western Australia with encouraging results.

Keywords: systems analysis, sensitivity analysis, simulation, Monte Carlo analysis, parametric uncertainty.

0301–4797/81/010007+12 $02.00/0

1. Introduction

The majority of environmental problems that have come to the public's notice in the last several decades have possessed the common characteristics of being scientifically quite complex yet requiring some governmental action for their alleviation in the short term. These characteristics have led to patterns of study and investigation of such problems in two major phases. Initially, large-scale literature searches are conducted, teams of specialists assembled and a variety of background studies begun. This first phase is then concluded by some form of assessment procedure which culminates in the specification of a strategy for the second phase of the study, an important feature of which is a detailed ordering of research priorities.

This paper is concerned with the scientific aspects of the assessment procedure and the process of establishing the second phase research priorities. In particular, we are interested in the suitability of mathematical models as vehicles for the organization of both qualitative and quantitative scientific data. We develop here a new method for examining a simulation model to determine whether it is capable of mimicking the salient qualitative aspects of the system behaviour that defines the environmental problem and, if so, to identify the segments of the model that are most important to a successful simulation. In this sense, the method is a generalized sensitivity analysis and can be used at an early stage of a research project to isolate the critical uncertainties in knowledge of the system and thereby to derive information of use in focusing the next phase of the research.

At the stage of the investigation with which we are here concerned, there is no alternative to utilizing some type of *simulation model* as the mathematical format into which assumptions regarding causal relations and parameter values are summarized. By *simulation model*, we mean one whose structure and parameters are explicitly related to physical, chemical or biological processes. Data in the literature on algal growth rates as a function of nutrient level, for example, are often given in terms of Michaelis constants, a fact which points out that simulation models are constrained to be written in the language of the various disciplines which have studied the component processes of the system. This constraint immediately leads to the result that most simulation models will be complex with many parameters, state variables and non-linear relations. Under the best circumstances, such models have many degrees of freedom and, with judicious fiddling, can be made to produce virtually any desired behaviour, often with both plausible structure and parameter values. Because of this problem, simulation modelling has limited importance in cases where extensive data sets that quantify the system behaviour are lacking.

In spite of the problems cited above, the potential utility of information yielded by simulation models in planning experiments has been recognized. For example, with reference to ecological models, Jeffers (1972) states that:

> "much time can be saved in the early stages of hypothesis formulation by the exploration of these hypotheses through mathematical models. Similarly mathematical models can be used readily to investigate phenomena from the viewpoint of existing theories, by the integration of disparate theories into a single working hypothesis, for example. Such models may quickly reveal inadequacies in the current theory and indicate gaps where new theory is required".

Similarly, Mar (1974) in his review of multidisciplinary modelling studies pointed out that:

> "The strategy to construct models without data and then employ sensitivity analysis to identify critical components where research and new data would enhance model performance is not commonly practised".

Stenseth (1977), while roundly criticizing simulation modelling, admits that a simple model, when used to explore or to generate hypotheses, can be a valuable research tool. Unfortunately, little work has been done to elucidate exactly how mathematical models can actually be used in such a "hypothesis generating" mode.

Several workers (e.g. Adams, 1972; Meyer, 1972; Maddock, 1973; McCuen, 1976) have suggested that parameter sensitivity analysis can be used to guide future data collection efforts and/or to order research priorities. Traditional parameter sensitivity analysis, however, pertains to a particular point in the parameter space (the vector space spanned by all possible combinations of parameter values). This requires that point estimates of all parameters be available, which, in turn, for complex environmental models, implies that sufficient input–output data for model calibration exist, and this is counter to our original premise that application was to be for an early stage of the investigation. Although Meyer (1972) advocates the use of a "tentatively calibrated model" to overcome this particular dilemma, the structure of models of environmental systems is not likely to be well defined *a priori*, and such an approach is therefore suspect.

In light of the discussion above, we contend that, in the early stages of the analysis of real problems, simulation models can be useful only in a probabilistic context. That is, given the model and the inherent uncertainties in structure and parameter values, the only meaningful analysis must focus on the probabilities of various behaviours. Most importantly, it must focus on the probable structures and parametric relations which appear consistent with that behaviour which is associated with the "environmental problem" under consideration. One method for applying simulation models in a probabilistic context is to use Monte-Carlo techniques. (For example, see Tiwari and Hobbie (1976*a*, *b*) and Tiwari *et al.* (1978) for an application of Monte-Carlo simulation in ecological modelling.) The methodology developed below adjoins the notion of qualitative or semi-quantitative descriptors of the *behaviour* of the system to Monte-Carlo simulation to obtain a useful technique for the preliminary analysis of environmental systems.

2. Class of mathematical models considered

For clarity of exposition, we restrict our attention to a specific class of models and introduce nomenclature which will be required subsequently. Assume the processes are to be modelled by a set of first order ordinary differential equations. (Different mathematical structures can be dealt with in an analogous way.) Let these equations be given in the form:

$$\frac{dx(t)}{dt} = \dot{x}(t) = f[x(t), \xi, z(t)] \tag{1}$$

where $x(t)$ is the state vector and $z(t)$ a set of time variable functions which include input or forcing functions. The vector ξ is a set of constant parameters described more fully below. Thus, for ξ, $z(t)$ and $x(0)$ specified, $x(t)$ is the solution of the system of equations and is a deterministic or a stochastic function of time as determined by the nature of $z(t)$. For simplicity of exposition, $z(t)$ will be treated hereafter as a deterministic function of t. Under this assumption, there are two types of uncertainty with which we will deal: uncertainty in the model structure, i.e. in the functions, f, and uncertainty in the parameter values, ξ. Different model structures would pertain to competing hypotheses on system functioning (e.g. phosphorus limitation versus nitrogen limitation in a eutrophication problem); we use the term *scenario* to indicate a particular structure.

For a given scenario, each element of the vector ξ is defined as a random variable the distribution of which is a measure of our uncertainty in the "real" but unknown value of the parameter. These parameter distributions are formed from data available from the literature and from experience with similar structures. For example, the literature suggests that the maximum growth rate of *Chlorella vulgaris* is almost certainly between 1·5 and 2·5 days^{-1} at water temperatures near 25°C. Interpreting these limits as the range of a rectangularly distributed random variable, and forming similar *a priori* estimates for the other elements of ξ result in the definition of an ensemble of models for a given scenario. Some of these models will, we hope, mimic the real system with respect to the behaviour of interest.

3. The problem-defining behaviour

Turning now to the question of behaviour, recall that, for a given scenario, every sample value of ξ, drawn from the *a priori* distribution, results in a unique state trajectory, $x(t)$. Following the usual practice, we assume that there are a set of observed variables $y(t)$, calculable from the state vector, which are important to the problem at hand. So, for each randomly chosen parameter set ξ^*, there corresponds a unique observation vector $y^*(t)$. Since the elements of $y(t)$ are observed (that is we assume that they are measured in the real system), it is sensible to define behaviour in terms of $y(t)$. For example, suppose y_t is the concentration of phytoplankton in a body of water and the problem in question concerns unwanted algal blooms due to nutrient enrichment. Then, there is some value of y_t above which a bloom is defined to have occurred and the behaviour is defined by this critical value.

In general, a number of behaviour categories can be used. Without loss of generality, however, we can consider the case for which behaviour is defined in a binary sense, i.e. it either occurs or does not occur for a given scenario and set of parameters ξ. It follows that a rule must be specified for determining the occurrence or non-occurrence of the behaviour on the basis of the pattern of $y(t)$. It is also possible that the behaviour might depend on the vector $z(t)$. For example, suppose one element of $z(t)$ was water temperature. We might be interested only in extreme values of $y(t)$ when adjusted or controlled for temperature variations. In any event, the detailed definition of behaviour is problem–dependent and, for present purposes, it is sufficient to keep in mind that a set of numerical values of ξ leads to a unique time function $y(t)$ which, in turn, determines the occurrence or non-occurrence of the behaviour conditioned, perhaps, by $z(t)$.

4. A generalized sensitivity analysis procedure

We have now presented the class of models to be studied, defined the scenario concept and described how we propose to deal with parametric uncertainty. For a given scenario, behaviour and set of parameter distributions ξ, it is possible to explore the properties of the ensemble via computer simulation studies. In particular, a random choice of the parameter vector ξ from the predefined distributions leads to a state trajectory $x(t)$, an observation vector $y(t)$ and, via the behaviour–defining algorithm, to a determination of the occurrence or non-occurrence of the behaviour. A repetition of this process for many sets of randomly chosen parameters results in a set of sample parameter vectors for which the behaviour was observed and a set for which the behaviour was not observed. The key idea is then to attempt to identify the subset of physically, chemically or biologically meaningful parameters which appear to account for the occurrence or

non-occurrence of the behaviour. More traditional sensitivity analyses of large ecological models inevitably show that a surprisingly large fraction of the total number of parameters is simply unimportant to the critical model behaviour. We maintain that this unimportant subset or, conversely, the critical subset, may be tentatively specified rather early in any study.

Ranking the elements of ξ in order of importance in the behavioural context is accomplished through an analysis of the Monte-Carlo results. The essential concept can best be illustrated by considering a single element, ξ_k, of the vector ξ and its *a priori* cumulative distribution, as shown in Figure 1. Recall that the procedure is to draw a

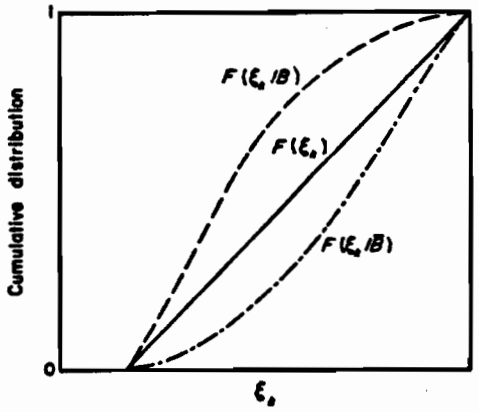

Figure 1. Cumulative distribution functions for parameter ξ_k. $F(\xi_k)$ = parent, *a priori* distribution, $F(\xi_k|B)$ = distribution of ξ_k in the behaviour category, $F(\xi_k|\bar{B})$ = distribution of ξ_k in the non-behaviour category.

random sample from this parent distribution (a similar procedure is followed for all other elements of ξ), run the simulation with this value and record the observed behaviour and the total vector ξ therewith associated. A repetition of this procedure results in two sets of values of ξ_k, one associated with the occurrence of the behaviour B, and the other without the behaviour $\bar{B}$. That is, we have split the distribution $F(\xi_k)$ into two parts as indicated in the figure. This particular example would suggest that ξ_k was important to the behaviour since $F(\xi_k)$ is clearly divided by the behavioural classification. Alternatively, if the sample values under B and $\bar{B}$ appeared both to be from the original distribution $F(\xi_k)$, then we would conclude that ξ_k was not important.

5. Sensitivity ranking of parameters

For the case where $z(t)$ is a deterministic function of time, the parameter space is cleanly divided by the behavioural mapping; that is, there is no ambiguity regarding whether a given parameter vector results in B or $\bar{B}$. Our analysis then focuses on the determination of which parameters or combinations of parameters are most important in distinguishing between B and $\bar{B}$. We will restrict the discussion to the case for which the parameter vector mean is zero and the parameter covariance matrix is the identity matrix. (A suitable transformation can always be found to convert the general problem to this case.) The problem of identifying how the behavioural mapping separates the parent parameter space can then be approached by examining induced mean shifts and induced covariance structure.

For example, we can base a sensitivity ranking on a direct measure of the separation of the cumulative distribution functions, $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$. In particular, we utilize the statistic:

$$d_{m,n} = \sup_x \left| S_n(x) - S_m(x) \right|$$

where S_n and S_m are the sample distribution functions corresponding to $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$ for n behaviours and m non-behaviours. The statistic $d_{m,n}$ is that used in the Kolmogorov–Smirnov two sample test and both its asymtotic and small sample distributions are known for any continuous cumulative distribution function $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$. Since S_n and S_m are estimates of $F(\xi_k|B)$ and $F(\xi_k|\bar{B})$, we see that $d_{m,n}$ is the maximum vertical distance between these two curves and the statistic is, therefore, sensitive not only to differences in central tendency but to any difference in the distribution functions. Thus, large values of $d_{m,n}$ indicate that the parameter is important for simulating the behaviour and, at least in cases where induced covariance is small, the converse is true for small values of that statistic.

In general, however, ranking on the basis of the separation in the distribution functions along the original axes of the parameter space (the individual parameter values) is not sufficient. It is possible, for example, that the first and second moments for a single parameter might exhibit no separation and yet this parameter could be crucial to a successful simulation by virtue of a strong correlation with other parameters under the behaviour. For example, Figure 2 depicts a two-dimensional parameter space for which

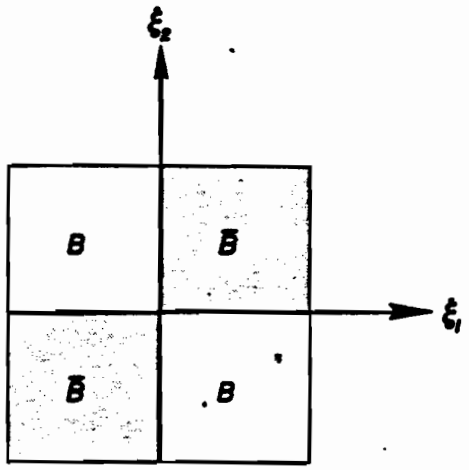

Figure 2. Schematic diagram of a two parameter case for which separation under the behavioural classification is total but for which discrimination by univariate tests is not possible.

the cumulative distributions would not separate under the behavioural classification. Nevertheless, both parameters are important in determining whether the behaviour occurs. Clearly, it is the interaction between parameters which is crucial, and information on the covariance between the two parameters will give insight into the degree of sensitivity in a case such as this. In fact, as shown more formally below, inspection of the

covariance matrices of the parameter vectors in the two classes can provide important clues in assessing sensitivity.

This notion can be formalized as follows. Let ξ be the parameter vector. Since these vectors were normalized to have zero mean, unity variance and zero covariance, it follows that:

$$E(\xi\,\xi^T) = I = P(B)E(Z_1 Z_1^T) + P(B)\mu_1\,\mu_1^T + P(\bar{B})E(Z_2 Z_2^T) + P(\bar{B})\mu_2\,\mu_2^T \qquad (2)$$

where:

$P(B)$ and $P(\bar{B})$ are probabilities of obtaining the behaviour and of not doing so, respectively

ξ_1 is a parameter vector associated with B

ξ_2 is a parameter vector associated with $\bar{B}$

$\mu_1 = E(\xi_1)$

$\mu_2 = E(\xi_2)$

$Z_1 = \xi_1 - \mu_1$

$Z_2 = \xi_2 - \mu_2$

E is the expectation operator.

The case illustrated in Figure 2 suggests that incidences in which separation is not indicated in the univariate analyses should be singled out in the multivariate procedure. Assume that m of the distributions $F(\xi_k)$ did not separate under the behavioural mapping. Then $\mu_{1k} = \mu_{2k} = 0$ for each of these distributions. For two parameters for which no mean shift is observed (say ξ_i and ξ_j), the ijth elements of $\mu_1\,\mu_1^T$ and $\mu_2\,\mu_2^T$ are zero and, according to equation (2), the corresponding off-diagonal elements of the covariance matrices are such that:

$$P(B)E(Z_{1i}Z_{1j}) = -P(\bar{B})E(Z_{2i}Z_{2j})$$

where $i \neq j$. Therefore, if a distribution does not separate under the behavioural mapping but does show induced covariance, the situation depicted in Figure 2, this covariance will be seen in both the covariance matrices under B and $\bar{B}$ and the magnitudes of the covariances will be related as indicated above. This is easily checked by inspection of the two matrices.

The problem of identifying "important" parameters in a situation where induced covariance is significant (e.g. the case shown schematically in Figure 2) can also be addressed by considering an analogy with the problem of discriminant analysis in the face of negligible differences in mean between groups. Kendall and Stuart (1969) suggest that a principal components transformation may be useful for such problems. In fact, for the case depicted in Figure 2 it is intuitively obvious that the principal components of the covariance matrix of parameters in the behaviour class (or of those in the non-behaviour class) define a new set of co-ordinate axes at 45° from the original ξ_1, ξ_2 axes. The cumulative distributions of the projections of the parameter vectors on these principal axes would indeed separate, and the value of the $d_{m,n}$ statistic for these would again provide a useful measure of the separation.

In a more general case, the behavioural classification would result both in separation along some of the original axes and in induced covariance. A principal components transformation of the covariance matrix of either the behaviour class or the non-behaviour class *defined with respect to the grand mean* can be used to advantage

when information on both mean and covariance differences is important (Fukunaga and Koontz, 1970). That is, equation (2) can be written:

$$E(\xi\xi^T) = I = P(B)E(\xi_1\xi_1^T) + P(\bar{B})E(\xi_2\xi_2^T)$$

and, if T is the matrix that diagonalizes the covariance matrix under the behaviour, $E(\xi_1\xi_1^T)$, then the same transformation must diagonalize the covariance matrix under the non-behaviour classification, $E(\xi_2\xi_2^T)$:

$$T^T E(\xi\xi^T)T = I = P(B)T^T E(\xi_1\xi_1^T)T + P(\bar{B})T^T E(\xi_2\xi_2^T)T, \text{ or}$$

$$I = P(B)\Lambda_1 + P(\bar{B})\Lambda_2 \qquad (4)$$

where Λ_1 and Λ_2 are diagonal matrices with the eigenvalues of the respective covariance matrices as the diagonal elements. The columns of the matrix T are eigenvectors of the covariance matrices, and the (normalized) components of those vectors are the direction cosines of the transformed axes relative to the original parameter axes. Thus, if the projections of the parameters on to a transformed axis exhibit significant separation under the classification in terms of the $d_{m,n}$ statistic, the weights on individual parameters in that eigenvector indicate the importance of each parameter in explaining the separation.

A simple example can be used to illustrate the general procedure. Figure 3 depicts a three-dimensional parameter space in which the univariate analysis should indicate

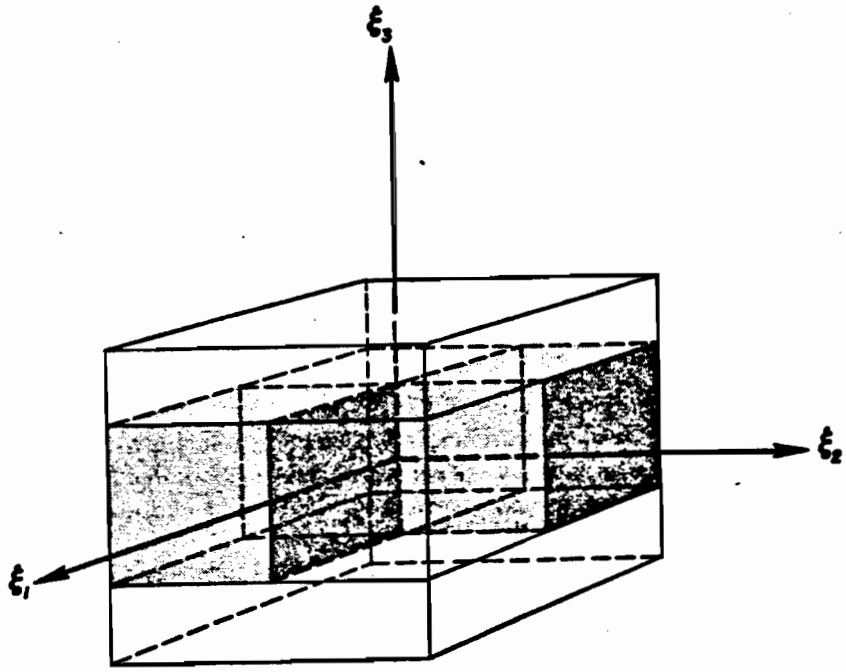

Figure 3. Diagram of a three parameter space. Parameter values in the shaded regions are defined to be in class B; those in the unshaded regions are defined to be in class $\bar{B}$.

separation on the ξ_3 axis but should not isolate the separation due to induced covariance in the $\xi_1\xi_2$ plane. Five hundred samples of parameter vectors were generated using random numbers and classified according to the scheme shown in Figure 3.

The univariate analysis of these vectors showed a $d_{m,n}$ of 0·09, 0·08 and 0·56 for ξ_1, ξ_2 and ξ_3 respectively. The first two are not significant at the 90% level whereas the last is significant at well above the 99% level.

The correlation matrices under the behaviour and non-behaviour are:

$$C(B) = \begin{bmatrix} 1{\cdot}00 & -0{\cdot}34 & 0{\cdot}05 \\ -0{\cdot}34 & 1{\cdot}00 & -0{\cdot}08 \\ 0{\cdot}05 & -0{\cdot}08 & 1{\cdot}00 \end{bmatrix}; \quad C(\bar{B}) = \begin{bmatrix} 1{\cdot}00 & 0{\cdot}40 & -0{\cdot}04 \\ 0{\cdot}40 & 1{\cdot}00 & 0{\cdot}0 \\ -0{\cdot}04 & 0{\cdot}0 & 1{\cdot}00 \end{bmatrix}.$$

As expected, there is a large correlation between the ξ_1 and ξ_2 parameters. Further, the off-diagonal elements of $C(B)$ and $C(\bar{B})$ are approximately of equal magnitude and of opposite sign. These large correlations between variables for which no univariate separation was seen suggest a principal components analysis as outlined above. Carrying out this analysis yields the eigenvectors of the matrix $E(\xi_1 \xi_1^T)$, which are the columns of the T matrix and, for this example, are:

$$T = \begin{bmatrix} -0{\cdot}72 & -0{\cdot}00 & -0{\cdot}070 \\ -0{\cdot}70 & -0{\cdot}00 & -0{\cdot}72 \\ -0{\cdot}00 & -1{\cdot}00 & -0{\cdot}00 \end{bmatrix}$$

The $d_{m,n}$ statistics are 0·18, 0·56 and 0·24 for the three eigenvectors. The second eigenvector (column 2) is, of course, the ξ_3 axis and reflects the mean separation in the original co-ordinates. The $d_{m,n}$ statistics for the other two directions are now significant at above the 99% level and the magnitude of the direction cosines in the $\xi_1 \xi_2$ plane ($\sim 0{\cdot}7$) indicates the equal importance of each of these original parameters in explaining this separation.

6. Application of the methodology

As one example of the application of the proposed method for preliminary analysis of environmental systems, we consider a problem of cultural eutrophication in a coastal plain estuary in Western Australia. Over the last decade, the Peel Inlet near Perth has been plagued by excessive growth of benthic alga *Cladophora* aff. *albida*. In 1976, the Estuarine and Marine Advisory Committee of the Environmental Protection Authority of Western Australia organized a consortium of academic and governmental research groups to assist in collecting data and developing the strategy necessary for the long-term management of the *Cladophora* nuisance.

The nature and extent of data available for Peel Inlet are such that the quantitative aspects of a conventional modelling exercise would not be of benefit. However, the information on similar types of problems reported in the open literature, coupled with the preliminary data from a survey of seasonal changes in *Cladophora* biomass and nutrient concentrations in Peel Inlet conducted by Dr A. J. McComb and his associates from the Botany Department of the University of Western Australia (Atkins *et al.*, 1977), provide enough information for applying the method we propose.

We chose to investigate a phosphorus scenario, and, in addition to the *Cladophora* compartment, included in the model compartments for phosphorus in the water column, in the sediment and in phytoplankton. The model included 19 parameters. The six criteria for defining the behaviour derived from the survey data in Atkins *et al.* (1977) and included limits for a *Cladophora* "bloom", timing of peak biomass, and maximum

concentrations of phytoplankton and dissolved phosphorus concentrations during the "bloom". A full description of the model of the behaviour criteria is given by Hornberger and Spear (1980).

Of 626 simulation runs conducted in the Monte-Carlo experiments, 281 fell in the behaviour category with 345 in the non-behaviour class. Sample distribution functions under B and $\bar{B}$ for two of the 19 parameters are shown in Figure 4. The Kolmogorov–Smirnov statistic, d_{mn}; = 0·20, indicates that $F(\gamma_1|B) \neq F(\gamma_1|\bar{B})$ at well above the 99% level of significance. The distributions of the light shading coefficient, k, on the other

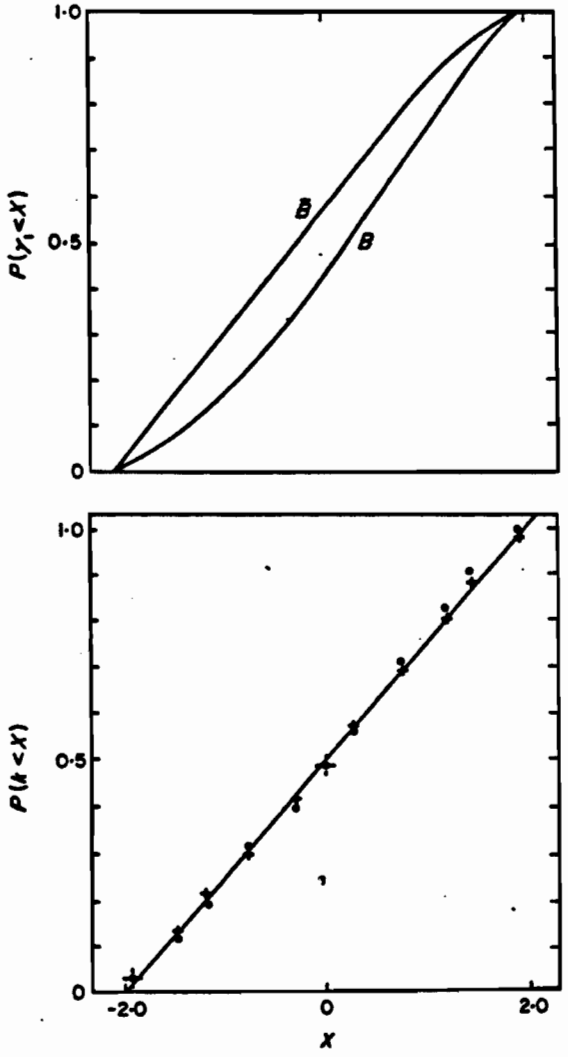

Figure 4. Cumulative distribution functions under the behavioural classification for (*a*) χ_1, Cladophora growth coefficient, which showed a distinct separation and (*b*) k, phytoplankton shading coefficient, which showed no significant separation. ●, $-\bar{B}$; +, $-B$.

hand, differ by a maximum of 0·05, a value which corresponds to a level of significance well below 90%. We interpret these results to indicate that γ_1 is an important determinant of the behaviour and k is not, at least in terms of a univariate analysis. A ranking of individual parameters on this basis classified seven of the 19 parameters as unimportant

for mimicking the behaviour and, as discussed below, isolated one set of processes as the critical linkage for successful simulation.

The analysis of induced covariance in this particular example indicated that all of the significant information on discrimination between groups was contained in the univariate analysis. The induced correlations between the parameters under the behavioural classification were, in general, small. The largest off-diagonal element of the correlation matrix was 0·23 and most were less than 0·1. Principal components analysis of the induced covariance showed that the vast majority of the discriminating information for the Peel Inlet problem is concentrated in mean shifts and can be determined directly from a ranking of the $d_{m,n}$ values for the individual parameters. The value of $d_{m,n}$ for the distributions projected on to the axis connecting μ_1 and μ_2 (i.e. the line connecting the centroid of the region associated with B and that associated with $\bar{B}$) was 0·56, roughly twice the largest value for a single parameter.

7. Discussion

We have developed a method for preliminary analysis of environmental systems that makes it possible to utilize a simulation model in conjunction with data from the literature and any available data for the system itself to determine areas of critical uncertainty. For example, the results of the Peel Inlet study described above indicated that the phosphorus scenario provides a feasible explanation of the nuisance algal problem if *Cladophora* have access to phosphorus in the sediment and if significant quantities of sediment-bound phosphorus are carried into the growth area by the Murray River (Hornberger and Spear, 1980; Spear and Hornberger, 1980). Critical uncertainties, as indicated by the statistical analyses, were associated with this supply of nutrient from sediments. Options for environmental management would obviously be tightly proscribed if the hypothesis generated by the preliminary analysis is true, and we concluded in an earlier report (Spear and Hornberger, 1980) that work should be initiated to test the hypothesis by quantifying the river input of sediment-bound nutrient, by establishing the extent to which this sediment is deposited in the areas where *Cladophora* are prominent, and by determining the rates of transfer of available phosphorus from the sediment to where the algae can utilize it.

As indicated above, the separation under the behavioural classification may not be so dominated by mean shifts in all problems. For example, we are currently applying our generalized sensitivity method to the model of the evolution of the earth's atmosphere proposed by Hart (1978). In this instance, the "correct" behaviour requires that the atmosphere evolve along lines that lead to approximately the present composition, temperature, etc. This requires that the successful simulation avoids "runaway glaciation" on the one hand and a "runaway greenhouse" on the other. We expect then that the parameters that lead to $\bar{B}$ may be on "both sides" of parameters that lead to B and that induced covariance may very well prove to be of considerable importance relative to mean shifts.

In addition to the obvious utility of the methodology to ordering research priorities, we feel that there is an even more direct link to environmental management. In any complex environmental system, only a relatively few processes are amenable to control. This fact can be used to examine management alternatives by augmenting the simulation model to include a set of "control" parameters and by performing the analysis with the full set of parameters. In this way, important control parameters can be isolated and the linkage with process parameters studied to formulate experiments to test control procedures. We are currently exploring this expanded use of the technique.

In concluding, we wish to emphasize that the approach we advocate is not equivalent to the typical simulation modelling effort and that we do not necessarily view it as a precursor to such an effort. Simulation modelling of environmental systems for purposes of management has been widely criticized (e.g. Hedgpeth, 1977; Young, 1977) and we feel that much of this criticism is justified. The methodology developed in this paper avoids the problems inherent in the use of simulation models as deterministic predictors, by concentrating on the probability of obtaining a result that is consistent with qualitative aspects of the behaviour under a full range of parameter uncertainty. Thus, it provides the basis for making practical use of simulation models in the field of environmental management.

References

Adams, W. M. (1972). Using the distributions observed in a simulation model of a flood-warning system to assign relative weights to research objectives. *Proc. Int. Symp. on Uncertainties in Hydrologic and Wat. Resour. Systems*, Univ. of Arizona, Tuscon, Arizona.

Atkins, R. P., Gordon, D. M., McComb, A. J. and Pate, J. S. (1977). Botanical contribution to the Peel/Harvey estuarine study. *Preliminary Rep. of Results Obtained During the First Year of the Study*. Dept. of Botany, Univ. of Western Australia, Perth.

Fukunaga, K. and Koontz, W. L. G. (1970). Application of the Karhunen–Loeve expansion to feature selection and ordering. *IEEE Trans. on Computers* **C-19**, 311–318.

Hart, M. H. (1978). The evolution of the atmosphere of the earth. *Icarus* **33**, 23–39.

Hedgpeth, J. W. (1977). Models and muddles. *Helgolander wiss. Meeresunters* **30**, 92–104.

Hornberger, G. M. and Spear, R. C. (1980). Eutrophication in Peel Inlet. I. The problem-defining behavior and a mathematical model for the phosphorus scenario. *Wat. Research* **14**, 29–42.

Jeffers, J. N. R. (1972). The challenge of modern mathematics to the ecologist. In *Mathematical Models in Ecology* (J. N. R. Jeffers, ed.). Oxford: Blackwell Scientific.

Kendall, M. G. and Stuart, A. (1969). *The Advanced Theory of Statistics. Vol. 3*. High Wycombe: Griffin.

Maddock, T., III. (1973). Management model as a tool for studying the worth of data. *Wat. Resour. Res.* **9**, 270–280.

Mar, B. W. (1974). Problems encountered in multidisciplinary resources and simulation models development. *J. Environ. Mgmt* **2**, 83–100.

McCuen, R. H. (1976). The anatomy of the modelling process. In *Mathematical Models for Environmental Problems* (C. A. Brebbia, ed.). London: Pentech Press.

Meyer, C. F. (1972). Surrogate modeling. *Wat. Resour. Res.* **8**, 212–216.

Spear, R. C. and Hornberger, G. M. (1980). Eutrophication in Peel Inlet. II. Identification of critical uncertainties via generalized sensitivity analysis. *Wat. Research* **14**, 43–49.

Stenseth, N. C. (1977). Modeling the population dynamics of voles: models as research tools. *Oikos* **29**, 449–456.

Tiwari, J. L. and Hobbie, J. E. (1976*a*). Random differential equations as models of ecosystems: Monte-Carlo simulation approach. *Math. Biosci.* **28**, 25–44.

Tiwari, J. L. and Hobbie, J. E. (1976*b*). Random differential equations as models of ecosystems—II. Initial condition and parameter specifications in terms of maximum entropy distributions. *Math. Biosci.* **31**, 37–53.

Tiwari, J. L., Hobbie, J. E. and Petersen, B. J. (1978). Random differential equations as models of ecosystems—III. Bayesian inference for parameters. *Math. Biosci.* **38**, 247–258.

Young, P. C. (1977). A general theory of modeling for badly defined systems. *Pap. presented at IFIP Conf. Modeling Land, Air and Water Resources Systems*, Ghent, Belgium.

WATER RESOURCES RESEARCH, VOL. 19, NO. 5, PAGES 1266–1270, OCTOBER 1983

Control of DO Level in a River Under Uncertainty

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A previously developed regionalized sensitivity analysis for exposing critical uncertainties in models of environmental systems is extended to study control of systems for which there is a good deal of uncertainty in the mathematical model used to describe the appropriate physical, chemical, and biological processes. The method is based on a binary classification of Monte Carlo simulation results as being either satisfactory or unsatisfactory in terms of controller performance. Contrasts in parameters associated with the two classes are elucidated by statistical analysis. This allows the selection of a set of control parameters that maximizes the probability of acceptable behavior in the presence of uncertainty in process parameters. The method is applied to the problem of regulating the discharge from a lagoon with the object of preventing DO from falling below a predetermined standard. It was found that for this system the desired behavior of the controlled process can be achieved with a probability of 0.84 with a particularly simple controller design. Nevertheless, the results suggest that even modest levels of uncertainty in the process parameters can have a considerable effect on the controller performance and that additional attention should be devoted to the design of robust controllers for environmental systems.

INTRODUCTION

Over the past 10 or 15 years there has been a sustained interest in the application of control theory to water quality problems in river systems. Many of these investigations have focused on DO/BOD dynamics and have employed either distributed [*Tarassov et al.*, 1969] or lumped parameter models of one sort or another [*Kendrick et al.*, 1970; *Young and Beck*, 1974; *Ozunger and Perkins*, 1979]. The control methodologies applied to these models have included dynamic programing [*Naito et al.*, 1972], duality theory [*Varaiya*, 1972], differential game theory [*Ozunger and Perkins*, 1979], procedures based on pole placement [*Young and Beck*, 1974; *Gourishankar and Raman*, 1977], forms of hierarchical control [*Tamura*, 1974] and Monte Carlo methods [*Whitehead and Young*, 1979].

Singh [1975] pointed out that many of these approaches are characterized by the considerable computational burden required to implement the control scheme. He proposed a suboptimal control scheme with more modest computational requirements to deal with this practical problem, but the fact remains that much of the reported work is of principally theoretical interest. An exception is the work of *Young and Beck* [1974], who carried out field studies aimed at giving some insight into the adequacy of their modeling approach for control purposes. Their model was subsequently used, in a simplified form, for theoretical studies by *Singh* [1975], *Ozunger and Perkins* [1979], and *Gourishankar and Raman* [1977]. However, none of these authors included the "sustained sunlight" term that Young and Beck found necessary to account for photosynthetic activity in the river and which their data suggested to be important to the overall DO/BOD dynamics. This omission led us to speculate on the effect of uncertainty in model structure or in process parameter values on the design and/or operation of the rather elaborate control schemes that have been developed. In systems with major biological components, uncertainty must be regarded as the rule rather than the exception. To investigate this issue in the context of the DO/BOD problem, we chose to study the implications of parametric uncertainty on the rather practical approach to the single-reach control problem taken by *Young and Beck* [1974].

We carried their rejection of the optimal control approach one step further by assuming that the important practical issue was simply to keep the DO concentration in the reach above some minimum level. The issue, then, was to determine the likelihood that the controller would be able to maintain an acceptable DO level in the presence of significant parametric uncertainty and, furthermore, to identify the key sources of uncertainty that affect controller performance.

We have previously developed a regional sensitivity analysis procedure for exposing the critical uncertainties in models of environmental systems [*Spear and Hornberger*, 1980; *Hornberger and Spear*, 1981]. This procedure depends upon an ability to construct plausible model structures, to estimate broad ranges of parameter values from limited field data or from the literature, and to define, rather loosely, the system behavior that is associated with the environmental problem (e.g., see *Hornberger and Spear* [1980]). The last of these, the behavioral definition, is crucial to the method, and it is worth emphasizing that the defining algorithm need not be analytic: thresholds, topological conditions, logical conditions, etc. are all permissible.

The essential features of our sensitivity analysis procedure are based on the following assumptions.

1. The problem under investigation can be qualitatively characterized by specific patterns of system response that define the "behavior" of concern.

2. One or more mathematical models of the system can be developed based on the relevant physical, chemical, or biological mechanisms that are assumed to underlie the problem behavior.

3. These models can be parameterized by statistical distributions rather than point estimates as a means of incorporating the uncertainty in the "actual" values of the parameters.

If, in a particular case, these conditions can be met, it is

Paper number 3W1224.
0043-1397/83/003W-1224$05.00

possible to conduct a Monte Carlo simulation by randomly selecting a parameter set from the predefined multivariate distribution, integrating the system equations, and classifying each simulation run according to the occurrence or nonoccurrence of the problem defining behavior. A repetition of this procedure n times leads to the accumulation of n parameter vectors which led to the behavior B and $n-m$ which led to not-the-behavior $\bar{B}$. The essential idea concerns the separation of the a priori parameter distributions under the behavioral mapping. That is, given the a priori cumulative distribution for the parameter ξ_i as $F(\xi_i)$, the issue concerns the degree to which $F(\xi_i|B)$ differs from $F(\xi_i|\bar{B})$. Clearly, if $F(\xi_i|\bar{B}) = F(\xi_i|B) = F(\xi_i)$, then it would seem that the parameter ξ_i was not important in determining the occurrence or nonoccurrence of the behavior. It transpires that this is a sufficient but not necessary condition for insensitivity, but together with its elaborations it is the central notion of the approach.

In this report we extend the sensitivity concept to the study of control of parametrically ill-defined systems in the context of the DO/BOD problem. Here the binary classification notion of the sensitivity approach is retained in the form of adequate or inadequate system performance, i.e., whether or not the DO criterion can be met. The new feature is that the controller design problem has two parameter sets, those associated with the control algorithm which can be specified by the designer and those associated with the physical, chemical, or biological processes to be controlled. The former set will be referred to as control parameters and the latter set, which are assumed to be uncertainly known, will be called process parameters, in conformity with usual practice. The specific design problem is, for a given feedback control algorithm, to select a fixed set of control parameters that maximize the probability of acceptable behavior in the presence of uncertainty in the process parameters.

DESCRIPTION OF THE PROBLEM

As stated above, our point of departure is the model of a single river reach proposed by *Young and Beck* [1974]. A waste stream of constant strength and constant discharge flows into a lagoon. Releases from the lagoon to the river are to be scheduled such that dissolved oxygen in the river is not driven below a specified water quality standard (the behavioral criterion in our formulation) and such that the lagoon does not overflow nor fall below some minimum level.

The model for a reach of the River Cam given by Young and Beck is in terms of dissolved oxygen (DO) and biochemical oxygen demand (BOD):

$$\frac{dx_1}{dt} = -\left[a_1 + \frac{Q+Q_E}{V_m}\right]x_1 - a_2x_2 + \frac{Q}{V_m}C_1 + a_1C_s - D_B + a_4(I_k - \bar{I}) + \frac{Q_E}{V_m}C_E \quad (1)$$

$$\frac{dx_2}{dt} = -\left[a_2 + a_3 + \frac{Q+Q_E}{V_m}\right]x_2 + \frac{Q}{V_m}L + L_A + a_5(I_k - \bar{I}) + \frac{Q_E}{V_m}L_E \quad (2)$$

A simple mass balance on the lagoon yields a third equation:

$$\frac{dV_L}{dt} = Q_L - Q_E \quad (3)$$

where V_L is constrained to be less than some maximum value at which point $Q_E = Q_L$. Also, $V_L > 0$. The state variables, input variables, and process parameters are as follows:

- x_1 output (downstream) DO, mg l^{-1};
- x_2 output BOD, mg l^{-1};
- L input (upstream) BOD, mg l^{-1};
- C_1 input DO, mg l^{-1};
- C_s saturation concentration of DO, mg l^{-1};
- Q_E discharge from lagoon, m^3 d^{-1};
- Q river discharge, m^3 d^{-1};
- V_m mean volume of the reach, m^3;
- V_L lagoon volume, m^3;
- a_1 reaeration rate constant, day^{-1};
- a_2 BOD decay constant, day^{-1};
- a_3 sedimentation rate constant, day^{-1};
- L_A mean rate of addition of BOD to the reach by local runoff, mg l^{-1} d^{-1};
- D_B net rate of removal of DO from the reach due to various components of respiration, mg l^{-1} d^{-1};
- I_k a "sustained sunlight" term to account for the observed correlation between sunlight and high concentrations of DO and BOD, h/d;
- $\bar{I}$ the threshold level of the sustained sunlight effect, h/d;
- a_4 DO rate constant for the sustained sunlight term, mg l^{-1} h^{-1};
- a_5 BOD rate constant for the sustained sunlight effect, mg l^{-1} h^{-1};
- Q_L discharge to the lagoon, m^3 d^{-1};
- L_E BOD concentration of lagoon effluent, mg l^{-1};
- C_E DO concentration of lagoon effluent, mg l^{-1}.

The sustained sunlight term is

$$I_k = I_{k-1} + \frac{1}{\tau_s}\left(h_k\frac{(\theta_k - \bar{\theta})}{\bar{\theta}} - I_{k-1}\right) \quad (4)$$

where

- k time index;
- τ_s time constant of the low-pass filter, days;

TABLE 1. Process Parameter Means and Values of the Kolmogorov Statistic for Monte Carlo Runs

	Mean Value	$d_{m,n}$ Run 1	Run 2	Run 3
		Process Parameters		
a_1	0.2	0.096	0.205	0.375
a_2	0.32	0.293	0.284	0.317
D_B	0.5	0.183	0.109	0.216
a_4	0.31	0.102	0.146	0.159
a_5	0.32	0.129	0.124	0.099
C_E	2.0	0.115	0.102	0.142
L_E	20.0	0.154	0.232	0.141
$\bar{I}$	6.0	0.309	0.321	0.343
τ_s	4.0	0.138	0.099	0.125
V_m	15.1×10^4	0.148	0.184	0.375
Q_L	2.8×10^4	0.097	0.136	0.192
$\bar{\theta}$	8.0	0.297	0.311	0.687
		Control Parameters		
k_1	see text	0.219	0.093	fixed
k_2	see text	0.132	0.293	fixed
k_3	see text	0.094	0.104	fixed
y_r	see text	0.320	0.170	fixed
$\bar{x}_2$	see text	0.166	0.271	fixed
		95% Value of $d_{m,n}$		
		0.182	0.173	0.232

h_k period of sunlight during the kth day, hours;
θ river water temperature, °C;
$\bar{\theta}$ a mean water temperature, °C.

The process parameters associated with the model of the DO-BOD dynamics are listed in Table 1. (We followed *Young and Beck* [1974] and set $a_3 = 0$ and $L_A = 0$.)

The controlled variable in this problem is Q_E, the lagoon discharge, which must be positive or zero. The value of this variable was determined from a control law which uses state variable feedback on output DO and BOD and integral error on DO. The control law for positive flowrates is

$$Q_E = -[k_1(x_1 - y_r) + k_2(x_2 - \bar{x}_2) + k_3 x_3] \qquad (5)$$

where y_r is the dissolved oxygen set point, $\bar{x}_2$ is the mean BOD level in the stream, k_1, k_2, and k_3 are controller gain parameters, and x_3 is the integral error variable, defined by a third state equation,

$$dx_3/dt = x_1 - y_r$$

which was introduced by Young and Beck in order to control x_1 to the desired set point y_r. In our treatment we modified this equation such that only values of x_1 less than y_r are of concern, and

$$dx_3/dt = x_1 - y_r \qquad x_1 < y_r$$

$$dx_3/dt = 0 \qquad x_1 > y_r$$

Also, when x_1 rises above y_r, x_3 is reset to zero. The control parameters to be specified are then k_1, k_2, k_3, y_r, and $\bar{x}_2$.

The method for examining the robustness of the controller design is similar to that for performing a regional sensitivity analysis. A range of possible values for the process parameters listed in Table 1 is chosen to reflect the system uncertainty. In this instance we simply used a rectangular probability density with a range of ±25% of the listed values to characterize the process parameter distributions. An example of how these distributions are specified in practice is contained in the work of *Hornberger and Spear* [1980]. The control parameters, however, are not uncertainly known but are to be determined from a range of allowable or feasible values. If we are prepared to stipulate this range, then it is possible to treat both control and process parameters similarly as far as the mechanics of the Monte Carlo simulation are concerned. The interpretation of the results of the Monte Carlo procedure will, of course, be quite different for the control versus the process parameters, as will be seen. A broad range of values was used for the parameters of the control law: the a priori distributions for k_1, k_2, and k_3 were bounded by $[-2.0 \times 10^5, 0]$, $[0, 1.0 \times 10^5]$, and $[0, 1.0 \times 10^5]$, respectively. The distribution bounds on the set point parameters, y_r and $\bar{x}_2$, were taken to be [5.0, 8.0] and [5.0, 10.0], respectively. The stream standard for DO was taken as 5.0 mg/l. As indicated above, this value constitutes the behavioral definition. If during a simulation run, x_1 goes below 5.0 mg/l, the run is a nonbehavior and, conversely, if x_1 remains above 5.0 mg/l, the run is a behavior. Input data (i.e., time series for L, C_1, Q, h_k, and θ_k) for the 80 days of each simulation run were those for the River Cam as reported by *Beck* [1978].

As indicated above, given the foregoing model and data, it is possible to carry out a number of Monte Carlo simulations by randomly selecting a parameter set from the predefined distributions, integrating the systems equations over the 80-day period and classifying each simulation run according to the occurrence or nonoccurrence of the "behavior." In order to assess the benefits of control, however, it is necessary to know the behavioral probability in the absence of control. Many systems, of course, will not operate at all without control, but environmental systems will often do so. Therefore the first simulation runs assumed the waste stream to be discharged directly to the river. Once the probability of behavior of the uncontrolled system, $P(B_0)$, is estimated, the marginal benefit of control, $M_B = P(B) - P(B_0)$, can be found for various controller designs.

In each of the Monte Carlo runs described below, we chose to conduct 250 replications based largely on our previous experience that the statistical methods employed seem well-behaved for sample sizes of this magnitude and greater. In this study the principal statistic employed was the Kolmogorov statistic, $d_{m,n} = \sup |S_n(\xi_i) - S_m(\xi_i)|$, where the $S(\xi_i)$ are the sample distribution functions of the parameter ξ_i for n behavior and m nonbehaviors. Here, "well-behaved" implies that $d_{m,n}$ tends toward a relatively constant value for $n + m \cong 250$ and both n and m greater than 50 or so. Of course, the significance level associated with a given $d_{m,n}$ continues to change with m and n even though $d_{m,n}$ itself approaches a constant value as m and n get large. Hence we regard the $d_{m,n}$ corresponding to a 95% level of significance as a "threshold" of separation between $F(\xi_i|B)$ and $F(\xi_i|\bar{B})$ but beyond that the magnitude of $d_{m,n}$ is probably a better index of the degree of separation than any measure based on significance level.

RESULTS AND DISCUSSION

The initial Monte Carlo run of 250 replications was carried out with process parameter bounds of ±25% of the values shown in Table 1 and without control. There occurred 20 behaviors, resulting in an estimate of 0.08 for $P(B_0)$.

A second run of 250 replications (Table 1, run 1) was carried out with the process parameter bounds unaltered and the control parameter bounds as given above. The ranges for the gain parameters k_1, k_2, and k_3 contain the fixed set selected by Young and Beck on the basis of desirable pole locations for the linearized system. The rationale for such wide bounds on these parameters is simply to give the analysis ample opportunity to discover those portions of the control parameter space in which behaviors are particularly dense.

Of the 250 Monte Carlo runs, 85 were behaviors and 165 nonbehaviors ($P_B = 0.34$). The values of the Kolmogorov statistic given in Table 1 (run 1) indicated that four of the 13 process parameter distributions and two of the five control parameter distributions separated under the behavioral mapping at above the 95% level of significance ($d_{m,n} = 0.182$). These were a_2, D_B, $\bar{I}$, $\bar{\theta}$, and the control parameters k_1 and y_r. Among these process parameters, $d_{m,n}$ was approximately 0.300 for a_2, $\bar{I}$, and $\bar{\theta}$ and 0.183 for D_B, the latter value just marginally in excess of the 95% value of 0.182. Figure 1 shows smoothed versions of $S_n(a_2|B)$ and $S_m(a_2|\bar{B})$ to illustrate the separation of the distributions under the behavioral mapping.

From an inspection of the cumulative distributions for the control parameters it was found that the portion of the control parameter subspace in which a higher proportion of behaviors will be found is at the low end of both the k_1 distribution and the y_r distribution, with k_2, k_3, and $\bar{x}_2$ being of little apparent consequence. The correlation matrix under the behavior contained values generally less than 0.2 with some interesting exceptions occurring for $\bar{\theta}$ with the control parameters: 0.29 with k_1, −0.32 with k_2, and −0.31 with y_r.

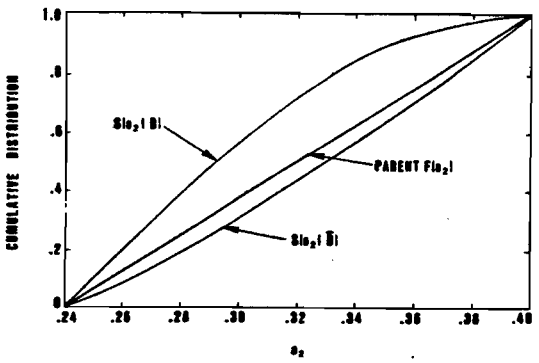

Fig. 1. The a priori distribution of parameter a_2 and smoothed sample distribution functions under the behavior B and not-the-behavior $\bar{B}$.

Utilizing the results of the previous run, the bounds for k_1 and y_r were altered to $[-2 \times 10^5, -1.5 \times 10^5]$ and [5, 6], respectively, for run 2. All other bounds were as before. These changes resulted in raising the behavior probability to 54% from the original 34%. The $d_{m,n}$ values are given in Table 1, run 2. In this region of parameter space there are some changes in the list of sensitive process parameters, with D_B dropping below the 95% significance level and a_1, L_E, and V_m appearing as important by virtue of rising above this level of significance. Of greater interest, however, are the changes in the control parameter sensitivities. As expected, k_1 and y_r become less important with $d_{m,n}$ values of 0.09 and 0.17, respectively. However, k_2 and $\bar{x}_2$ now have $d_{m,n}$ values of about 0.3. This result and the low correlation between the DO and BOD control parameters suggests that this region of control parameter space is good as far as the DO component of the controller is concerned but that further improvements are possible in the BOD component, i.e., k_2 and $\bar{x}_2$. As before, k_3 appears to be of little importance, which is not surprising in view of our behavioral definition. Hence, setting $k_3 = 0$ leads to a desirable simplification.

The distribution $S_n(k_2|B)$ indicates that behaviors are preferentially associated with values of k_2 on the low end of the range. As before, we might alter the k_2 distribution to cover the bottom 25% or so of the present range. Alternatively, we might recognize the practical fact that BOD analysis takes 5 days to accomplish and a scheme using x_2 feedback is not feasible for real time control purposes. The latter course leads to a choice of $k_2 = 0$ which, fortunately, is consistent with k_2 being at the low end of the range.

These choices simplify the design problem to that of choosing specific values for k_1 and y_r from the narrowed ranges given above. However, since neither the distribution of k_1 nor y_r separate under the behavioral mapping, the strategy used to arrive at the present region provides little further guidance. That is, it is knowledge of the fine structure of $F(k_1|B)$ and $F(y_r|B)$ that is necessary to obtain further information. To obtain such information is costly in terms of computer time, since large numbers of replications are required to obtain a good picture of the details of F from S_n. Before proceeding further on the practical questions, let us digress briefly to indicate what could be done with a good estimate of F if it were available.

We are seeking regions of the control parameter subspace in which the probability of behavior is high or, conversely, the probability of not-the-behavior is near zero. Let U be the event that the m-dimensional control parameter vector lies within a bounded region such that $a_i \le k_i \le b_i$ for $i = 1$, m where a_i and b_i lie within the limits of the rectangular distribution defined for k_i. Then

$$P(\bar{B}|U) = \frac{P(\bar{B})P(U|\bar{B})}{P(U)}$$

where $P(\bar{B})$ is the probability of not-the-behavior in the entire parameter space as originally defined. Since we assume each element of the control vector $\mathbf{k}$ is independently distributed,

$$P(U|\bar{B}) = \prod_{i=1}^{m} P(U_i|\bar{B})$$

where U_i is the event that $a_i \le k_i \le b_i$. Likewise,

$$P(U) = \prod_{i=1}^{m} P(U_i)$$

Since we desire to find the region U such that $P(\bar{B}|U) = 0$, this is equivalent to finding regions where

$$\prod_{i=1}^{m} P(U_i|\bar{B}) = 0$$

To locate this region we may inspect the cumulative distribution of each of the k_i under $\bar{B}$, since $P(U_i|\bar{B}) = F(b_i|\bar{B}) - F(a_i|\bar{B})$. That is, we are looking for "flat" places on each of the functions $F(k_i|\bar{B})$.

If the behavioral mapping had resulted in appreciable covariance among the elements of $\mathbf{k}(\bar{B})$, an analogous argument can be developed for dealing with a parameter set transformed by the matrix which diagonalizes the covariance matrix $E[(\mathbf{k} - \boldsymbol{\mu})(\mathbf{k} - \boldsymbol{\mu})^T]$ where $\boldsymbol{\mu} = E(\mathbf{k}|\bar{B})$.

Returning to the practical issue, one can either use $S_n(k_1|\bar{B})$ and $S_n(y_r|\bar{B})$ for $n = 250$ and assume that any apparent flat spots are real or carry out further runs to increase n. The choice clearly depends on the cost/benefit situation for the problem at hand. Here we take the former course and select $k_1 = -1.8 \times 10^5$ and $y_r = 5.4$. These values, together with $k_2 = k_3 = 0$, constitute a controller design which, in an additional 250 replications, resulted in an estimate of the behavioral probability of 0.84 (Table 1, run 3). We cannot contend that this is the best that can be done, but it is a design which raises the probability of keeping the DO in the stream above 5 mg/l from 0.08 without control to 0.84 with a particularly simple control scheme.

Under the above design conditions the occurrence of the behavior is sensitive to five process parameters. They are a_1, a_2, $\bar{I}$, V_m, and $\bar{\theta}$. Of these, $\bar{\theta}$ is overwhelmingly important with a $d_{m,n}$ of 0.687 as contrasted with the 95% value of 0.232. In fact, $S_n(\bar{\theta}|\bar{B})$ is zero until $\bar{\theta}$ is near its mean value. Hence, if in the real system the value of $\bar{\theta}$ is low, behaviors will be obtained with a probability very near to unity with this controller design.

CONCLUSION

The final result, then, is that with the defined inputs and the process parameter distributions the desired behavior of the controlled process can be achieved with a probability of 0.84 with a particularly simple controller design. If this probability were deemed insufficient, three courses of action are open, at least in theory: one might enlarge the lagoon thereby increasing the overall control capacity, one might engage in further research to narrow the process parameter uncertainty, or one might investigate other controller structures. In the case of

process uncertainty, the results of the analysis strongly suggest that algal photosynthetic activity is critical in that the distribution of the parameter $\bar{\theta}$ separated with a $d_{m,n}$ of 0.687 in the final Monte Carlo run as discussed above. The related parameter $\bar{I}$ also was marginally important.

Although we cannot argue that the ±25% variability assigned to the process parameters is "realistic," neither do we feel that it reflects an unrealistic degree of uncertainty for biological parameters in systems without real time estimation capability. Clearly, this degree of uncertainty has had a profound effect upon the controller design with which we began. Two of its three terms were dropped since they appeared to have little effect on the outcome. With DO feedback alone the controller is able to do quite a decent job of attaining the DO goal. A key result, however, is that two of the parameters associated with algal photosynthesis were critical to the controller's ability to maintain acceptable DO levels. That is, even with a rather modest control objective, the uncertainty in the process parameters strongly conditions the ability of the system to attain its goal. This result is, perhaps, not surprising, but it would seen to suggest that the design of robust controllers for such systems is a subject that deserves more attention than it has received in the past. The extension of the regionalized sensitivity analysis developed previously by *Spear and Hornberger* [1980] and *Hornberger and Spear* [1981] is one method for dealing with the design of robust controllers for uncertain environmental systems. The use of the method has already proved to be attractive for the design of controllers for well-defined processes where nonanalytic performance criteria are desirable or in cases where the process is nonlinear or otherwise analytically intractable [*Auslander et al.*, 1982]. We have shown here that the method retains this basic utility for natural environmental systems for which thoroughly validated and verified mathematical models are not available. It would appear that the general approach can be modified and elaborated to address a wide variety of practical problems.

Acknowledgments. This research was supported in part under NASA Cooperative Agreement NCC2-67 and carried out in part at the Institute of Hydrology, Wallingford, United Kingdom.

REFERENCES

Auslander, D. M., R. C. Spear, and G. E. Young, A simulation-based approach to the design of control systems with uncertain parameters, *J. Dyn. Syst. Meas. Control, 104*, 20–26, 1982.

Beck, B., A comparative case study of dynamic models for DO-BOD-algal interactions in a freshwater river, *Rep. RR-78-19*, Int. Inst. for Appl. Syst. Anal., Laxenburg, Austria, 1978.

Gourishankar, V., and K. Raman, Design of a water quality controller by pole placement, *IEEE Trans. Syst. Man Cybern., SMC7*, 109–111, 1977.

Hornberger, G. M., and R. C. Spear, Eutrophication in Peel Inlet, 1, The problem defining behavior and a mathematical model for the phosphorus scenario, *Water Res., 14*, 29–42, 1980.

Hornberger, G. M., and R. C. Spear, An approach to the preliminary analysis of environmental systems, *J. Environ. Manage., 12*, 7–18, 1981.

Kendrick, D. A., H. S. Rao, and C. H. Wells, Optimal operation of a system of waste water treatment facilities, paper presented at the Symposium on Adaptive Processes, Inst. of Electr. and Electron. Eng., New York, 1970.

Naito, M., T. Takamatsu, T. Fakuda, and H. Tamura, Optimum planning of sewage treatment systems for preserving stream quality, paper presented at the 5th Congress, Int. Fed. of Autom. Control, Paris, 1972.

Ozunger, U., and W. R. Perkins, A Nash feedback approach to the control of river pollution, *IEEE Trans. Systems Man Cybern., SMC9*, 290–292, 1979.

Singh, M. G., River pollution control, *Int. J. Syst. Sci., 6*, 9–21, 1975.

Spear, R. C., and G. M. Hornberger, Eutrophication in Peel Inlet, 2, Identification of Critical uncertainties via generalized sensitivity analysis, *Water Res., 14*, 43–49, 1980.

Tamura, H., A discrete dynamic model with distributed transport delays and its hierarchical optimization for preserving stream quality, *IEEE Trans. Systems Man Cybern., SMC4*, 424–431, 1974.

Tarassov, V. J., H. J. Perliss, and B. Davidson, Optimization of a class of river aeration problems by the use of multivariable distributed parameter control theory, *Water Resour. Res., 5*, 563–573, 1969.

Varaiya, P. P., *Notes on Optimization*, Van Nostrand, New York, 1972.

Young, P. C., and B. Beck, The modelling and control of water quality in a river system, *Automatica, 10*, 455–468, 1974.

Whitehead, P., and P. C. Young, Water quality in river systems: Monte Carlo analysis, *Water Resour. Res., 15*, 451–459, 1979.

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(Received February 14, 1983;
revised July 19, 1983;
accepted July 20, 1983.)

Selection of Parameter Values in Environmental Models Using Sparse Data: A Case Study

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ABSTRACT

Models of environmental processes must often be constructed without the use of extensive data sets. This can occur because the exercise is preliminary (aimed at guiding future data collection) or because requisite data are extremely difficult, expensive, or even impossible to obtain. In such cases traditional, statistically based methods for estimating parameters in the model cannot be applied; in fact, parameter estimation cannot be accomplished in a rigorous way at all. We examine the use of a regionalized sensitivity analysis procedure to select appropriate values for parameters in cases where only sparse, imprecise data are available. The utility of the method is examined in the context of equilibrium and dynamic models for describing water quality and hydrological data in a small catchment in Shehandoah National Park, Virginia. Results demonstrate that (1) models can be "tentatively calibrated" using this procedure; (2) the data most likely to provide a stringent test of the model can be identified; and (3) potential problems with model identifiability can be exposed in a preliminary analysis.

INTRODUCTION

Mathematical modeling of environmental systems is now a well-established practice. In certain instances problems are well defined, appropriate data can be collected, and statistical methods can be applied to ensure that inferences drawn from the model are supportable. In other instances the obverse situation may prevail: the problem is poorly defined, suitable data are lacking, and traditional statistical analyses either are impossible to perform or do not lead to any useful results. We are interested here in the utility of mathematical models in the latter situation.

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52 Vanderbilt Ave., New York, NY 10017 0096-3003/85/$03.30

We will refer to the class of models that we consider as *speculative simulation models*. By "simulation model" we mean one whose structure and parameters are explicitly related to physical, chemical, or biological processes. (In hydrology, the term "conceptual model" is generally used [5].) We append the qualifier "speculative" to indicate that, for cases with which we are concerned, available data, or at least portions of the data, are so sparse that rigorous calibration and validation of the models are not possible; we are interested in the analysis of "badly defined systems," as described in [28].

We believe that speculative simulation models, despite their wide use as predictive, deterministic representations of reality, are useful only in a probabilistic context. Specifically, because of uncertainty surrounding the entire conceptual basis of the model, we maintain that analysis should focus on the probable model structures and parameter values that appear to be consistent with available information. Our approach to such analysis is to use a methodology referred to here as a "regionalized sensitivity analysis" (RSA), first proposed in [26] and [11]. The method has proved useful in a number of studies of badly defined natural systems [10, 11, 26, 27, 1, 8, 7, 29, 13, 30, 6].

Research reported here deals with the application of the RSA to the problem of selecting parameter values for a particular model structure in the face of sparse and/or unavailable data. In particular, we apply the method to the problem of modeling hydrology and water chemistry in a small catchment in Shenandoah National Park, Virginia.

THE RSA PROCEDURE

The basis of the RSA method is the utilization of a simulation model together with a classification algorithm. The classification allows any particular trajectory of the state variables of the system generated by the model to be identified as either representative of the observed (or desired) behavior of the system or not representative of the behavior. The idea is to inject uncertainty into the simulation model of the system by specifying the parameters via probability density functions (rather than point estimates) and then to perform Monte Carlo simulations, choosing parameter values from the specified distributions. The result of each Monte Carlo replication is classified as either behavior, B, or nonbehavior, $\bar{B}$. Subsequent to the Monte Carlo trials, statistical analysis of the parameter vectors is used to isolate those parameters important in simulating the salient features defining the observed behavior. The sensitivity rankings of the parameters are taken to be indicative of the relative importance of uncertainties in various component processes.

Assume an environmental system to be modeled by a set of first order ordinary differential equations. Let these equations be given in the form

$$\frac{d\mathbf{x}(t)}{dt} = \dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \boldsymbol{\xi}, \mathbf{z}(t)),$$

where $\mathbf{x}(t)$ is the state vector and $\mathbf{z}(t)$ a set of time-variable functions which include input or forcing functions. The vector ξ is a set of constant parameters described more fully below. Thus for ξ, $\mathbf{z}(t)$, and $\mathbf{x}(0)$ specified, $\mathbf{x}(t)$ is the solution of the system of equations and is a deterministic or stochastic function of time as determined by the nature of $\mathbf{z}(t)$. For simplicity of exposition, $\mathbf{z}(t)$ will be treated hereafter as a deterministic function of t. Under this assumption, there are two types of uncertainty with which we will deal: uncertainty in the model structure, i.e. in the functions $\mathbf{f}$, and uncertainty in the parameter values ξ. Different model structures would pertain to competing hypotheses on system functioning. We use the term *scenario* to indicate a particular structure.

For a given scenario each element of the vector ξ is defined as a random variable, the distribution of which is a measure of our uncertainty in the "real" but unknown value of the parameter. These parameter distributions are formed from data available from the literature and from experience with similar structures. In most situations, the available data can best be used to give allowable *limits* of parameter values. Interpreting these limits as the range of a rectangularly distributed random variable for each element of ξ results in the definition of an ensemble of models for a given *scenario*. Some of these models will, we hope, mimic the real system with respect to the behavior of interest.

Turning now to the question of behavior, recall that for a given scenario every sample value of ξ, drawn from the *a priori* distribution, results in a unique state trajectory, $\mathbf{x}(t)$. Following the usual practice, we assume that there is a set of observed variables $\mathbf{y}(t)$, which can be calculated from the state vector important to the problem at hand. So, for each randomly chosen parameter set ξ^*, there corresponds a unique observation vector $\mathbf{y}^*(t)$. Since the elements of $\mathbf{y}(t)$ are observed (i.e., they are measured in the real system) it is sensible to define behavior in terms of $\mathbf{y}(t)$. For example, suppose y_i is the runoff in a given stream and the study relates to floods equaling or exceeding a given magnitude. The behavior in this case will be defined by the occurrence of a predicted discharge at or above the specified level.

In general a number of behavior categories can be used. In fitting rainfall-runoff models one might be interested in discerning differences among classes of response that: (1) matched a number of storms by total volume of discharge within some percentage difference *and* matched peak flows within some specified difference; (2) matched the peaks but not the volumes; (3) matched neither. That is, one might want to isolate modeled processes that were most important to a variety of modes of behavior. Without loss of generality, however, we can consider the case for which behavior is defined in a binary sense, that is, it either occurs or does not occur for a given scenario and set of parameters ξ.

We have now presented the class of models to be studied, defined the scenario concept, and described how we propose to deal with parametric

uncertainty. For a given scenario, behavior, and set of parameter distributions ξ, it is possible to explore the properties of the ensemble via computer simulation studies. In particular, a random choice of the parameter vector ξ from the predefined distributions leads to a state trajectory $\mathbf{x}(t)$, an observation vector $\mathbf{y}(t)$, and (via the behavior-defining algorithm) a determination of the occurrence or nonoccurrence of the behavior. A repetition of this process for many sets of randomly chosen parameters results in a set of sample parameter vectors for which the behavior was observed and a set for which the behavior was not observed. The key idea is then to attempt to identify the subset of physically, chemically, or biologically meaningful parameters which appear to account for the occurrence or nonoccurrence of the behavior. More traditional sensitivity analyses of large environmental models inevitably show that a surprisingly large fraction of the total number of parameters are simply unimportant to the critical model behavior. We maintain that this unimportant subset, or conversely the critical subset, may be tentatively specified in a reasonably objective fashion.

Ranking the elements of ξ in order of importance in the behavioral context is accomplished through an analysis of the Monte Carlo results. The essential concept can be best illustrated by considering a single element ξ_k of the vector ξ and its *a priori* cumulative distribution as shown in Figure 1. Recall that the procedure is to draw a random sample from this parent distribution (a similar procedure is followed for all other elements of ξ), run the simulation with this value, and record the observed behavior and the total vector ξ therewith associated. A repetition of this procedure results in two sets of values of ξ_k, one associated with the occurrence of the behavior B, and the other with nonbehavior $\bar{B}$. That is, we have split the distribution $F(\xi_k)$ into two parts as indicated in Figure 1. This particular example would suggest that ξ_k was important to the behavior, since $F(\xi_k)$ is clearly divided by the behavioral classification. Alternatively, if the sample values under B and $\bar{B}$ appeared both to be from the original distribution $F(\xi_k)$, then we would conclude that ξ_k was not important.

For the case where $\mathbf{z}(t)$ is a deterministic function of time, the parameter space is cleanly divided by the behavioral mapping; that is, there is no ambiguity regarding whether a given parameter vector results in B or $\bar{B}$. Our analysis then focuses on the determination of which parameters or combinations of parameters are most important in distinguishing between B and $\bar{B}$. We will restrict the discussion to the case for which the parameter vector mean is zero and the parameter covariance matrix is the identity matrix. (A suitable transformation can always be found to convert the general problem to this case.) The problem of identifying how the behavioral mapping separates the parent parameter space can then be approached by examining induced mean shifts and induced covariance structure.

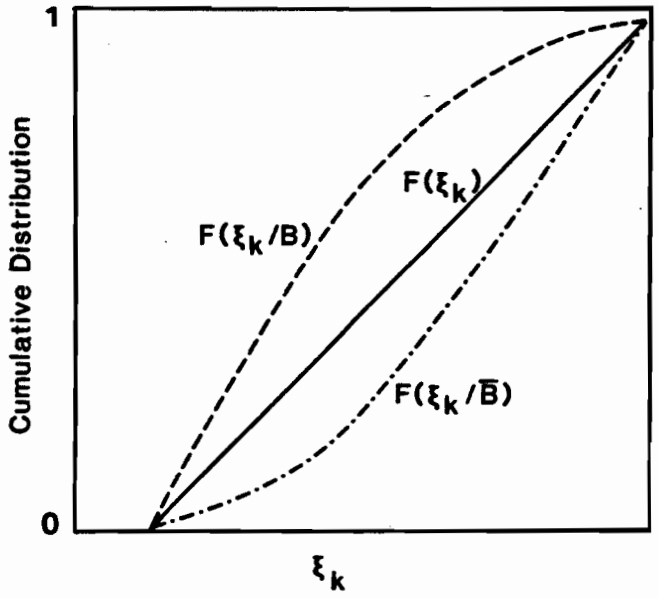

FIG. 1. Cumulative distribution functions for parameter ξ_k, where $F(\xi_k)$ = parent, *a priori* distribution, $F(\xi_k/B)$ = distribution of ξ_k in the behavior category, $F(\xi_k/\bar{B})$ = distribution of ξ_k in the nonbehavior category.

For example, we can base a sensitivity ranking on a direct measure of the separation of the cumulative distribution functions, $F(\xi_k/B)$ and $F(\xi_k/\bar{B})$. In particular, we utilize the statistic

$$d_{m,n} = \sup_x |S_n(x) - S_m(x)|,$$

where S_n and S_m are the sample distribution functions corresponding to $F(\xi_k/B)$ and $F(\xi_k/\bar{B})$ for n behaviors and m nonbehaviors. The statistic $d_{m,n}$ is that used in the Kolmogorov-Smirnov two sample test, and both its asymptotic and small sample distributions are known for any continuous cumulative distribution functions $F(\xi_k/B)$ and $F(\xi_k/\bar{B})$. Since S_n and S_m are estimates of $F(\xi_k/B)$ and $F(\xi_k/\bar{B})$, we see that $d_{m,n}$ is the maximum vertical distance between these two curves, and the statistic is therefore sensitive not only to differences in central tendency but to any difference in the distribution functions. Thus, large values of $d_{m,n}$ indicate that the parameter is important for simulating the behavior, and, at least in cases

where the induced covariance is small, the converse is true for small values of that statistic. For our purposes this analysis of univariate distributions suffices. Hornberger and Spear [11] describe the extension to cases where induced covariance is important.

APPLICATION OF THE PROCEDURE

One area in studies of natural environmental systems that has proven to be especially fertile for the development of simulation models is catchment dynamics. Eliciting a quantitative relationship between rainfall and runoff from catchments has been of great concern to environmental scientists throughout the modern period of the science of hydrology. The additional problem of accounting for chemical transformations of water as it passes through a catchment has also led to the development of hydrochemical simulation models in recent years. These models, be they purely hydrological or hydrochemical, *must* be speculative simulation models, inasmuch as even the most physically based of them cannot reflect the complexity and heterogeneity of processes as demonstrated in the field. Furthermore, the more complex the models become, the more difficult the problems of identification and parameter estimation become. Nevertheless, a host of important questions can only be approached via the application of simulation models to catchments. The RSA procedure can be put to good use in these applications.

The Shenandoah Watershed Acidification Study (SWAS), initiated in October 1979, focuses on processes in White Oak Run (WOR), a 5.15 km^2 forested catchment in Shenandoah National Park, Va. The purpose of the project is to estimate the probable past effects and the potential future effects of acid precipitation on soils and streams in the Park [23]. To this end we have examined the application of speculative simulation models to WOR. Below we describe two aspects of the study: a hydrological model and an equilibrium chemistry model.

HYDROLOGICAL MODELING

We use a model that derives from one used in a study by Beven and Kirkby [3]. This model is semidistributed in that it can predict the spread of a variable saturated contributing area on the basis of catchment topography and soil characteristics. The predicted patterns show a good resemblance to patterns of saturation measured in the field [3].

Beven and Wood [4] showed that the model could be further improved by taking into account the areal pattern of saturation storage deficits which may be predicted by the model in routing flow through the unsaturated zone. This

revised model gave good predictions of storm runoff volumes for several catchments, including WOR. The model can predict very different contributing areas for the same storm runoff, depending on catchment characteristics, storm rainfall distribution, and antecedent conditions.

We further extended the model to enable simulation of flows on a time-continuous basis in WOR. We included modifications that conceptually covered all types of hydrological behavior that were observed or inferred from field measurements [31, 32]. The final model contained 13 adjustable parameters. (See [9] and [12] for a complete description of the model.)

It is well known that calibration of rainfall-runoff models, especially when the model contains a rather large number of parameters and when the data available for calibration relate to whole catchment input-output, is problematic [14, 5, 15, 18, 17, 16, 25]. In most cases the instability of parameter estimates stems from the fact that the structural complexity of the model is greater than is warranted on the basis of the calibration data set; the model has "surplus content." The RSA procedure can be used to elucidate which processes in the model appear to be responsible for observed behavior and, conversely, which of the modeled processes appear to make little or no difference in model predictions.

In the case of rainfall-runoff modeling there are usually extensive input-output data sets available for calibration. For WOR, for example, we used approximately 1.5 years of 3 hourly measured values of precipitation and stream discharge in the calibration study. Why, then, should we consider this to be a situation with "sparse data"? For simulation models such as the modified Beven-Wood model which we employed, there are several unobserved states (e.g., soil moisture) intrinsic to the model. Observations of these states might greatly facilitate the calibration and testing of hydrological simulation models [16], but these data are not generally available.

The calibration is therefore most often implemented using only rainfall and runoff data, a procedure that we followed for WOR. The parameter values are selected on the basis of some goodness-of-fit criterion, an objective function such as the sum of squared errors between simulated and observed runoff. One of the advantages of the RSA procedure is that nonstandard objective functions can be used to define the behavioral classification. It is possible, for example, to define a behavior criterion that would consider a simulation successful if three-quarters of the predicted storm volumes were within 5% of measured values *and* the remaining predictions were within 15% of measured values. Examination of results from such unorthodox (but perhaps highly meaningful to field scientists) criteria can be very revealing in exposing how different portions of the simulation model work. To keep the discussion manageable, we report here results using two traditional objective functions to define the behavior categories: (1) the sum of squared errors (SSE) and (2)

the log likelihood function proposed by Sorooshian and Dracup [24]. For all optimizations we used the Rosenbrock [22] method.

In implementing the RSA procedure for the hydrology model, values of each parameter were selected randomly from uniform distributions over the physically meaningful ranges of the thirteen parameters. (If the parameter was one whose values can range over several orders of magnitude, we chose the logarithm of the parameter from a uniform distribution.) The model was run for the calibration period and the SSE calculated for that particular realization of the simulation model. After 330 realizations were accumulated, the distribution of parameter values for the lowest 30% of the SSE values was compared with the distribution of values for the highest 70%. The comparison was made using the Kolmogorov-Smirnov statistic $d_{m,n}$. If these distributions differed greatly, then the model output was deemed sensitive to that parameter (as measured by the SSE). If the difference between the distributions was small, however, the model output was deemed indifferent to the value of that parameter, so that any value within the prespecified range could be considered as "reasonable" as any other.

The model output was sensitive (as judged by the SSE) to only four of the thirteen model parameters. The cumulative distributions of these four parameters when the SSEs were in the lowest 30% differed significantly ($p = .01$) from the cumulative distributions of the parameters when the SSEs were in the highest 70% (Figure 2). If a statistical optimization of the parameter values (using SSE as the objective function) were attempted, we might expect that the response surface for the four sensitive parameters would be well behaved and that the optimization routine would converge to the same global optimum values of these four parameters regardless of the values of the nine insensitive parameters. Alternatively, we could interpret the RSA results as indicative of "surplus content" in the model and reduce the model structure by removing the processes represented by the insensitive parameters. The expectation in this case would be that the response surface of the reduced model would be better behaved than that of the full model and the global convergence of the optimization routine would be improved. We examine both premises.

The Rosenbrock routine was used to select "optimal" values for the thirteen parameters in the full model. Starting values for each parameter to be used in the iterative routine were chosen at random from the ranges of parameter values used in the RSA. This procedure was repeated ten times to determine whether the optimization procedure (based on SSE) consistently converged to unique "optimal" values of the four sensitive parameters and whether the final SSEs of each optimization run were similar (i.e. the routine converges to a global minimum SSE regardless of the values of the insensitive parameters). The SSEs for these random starting point optimizations ranged

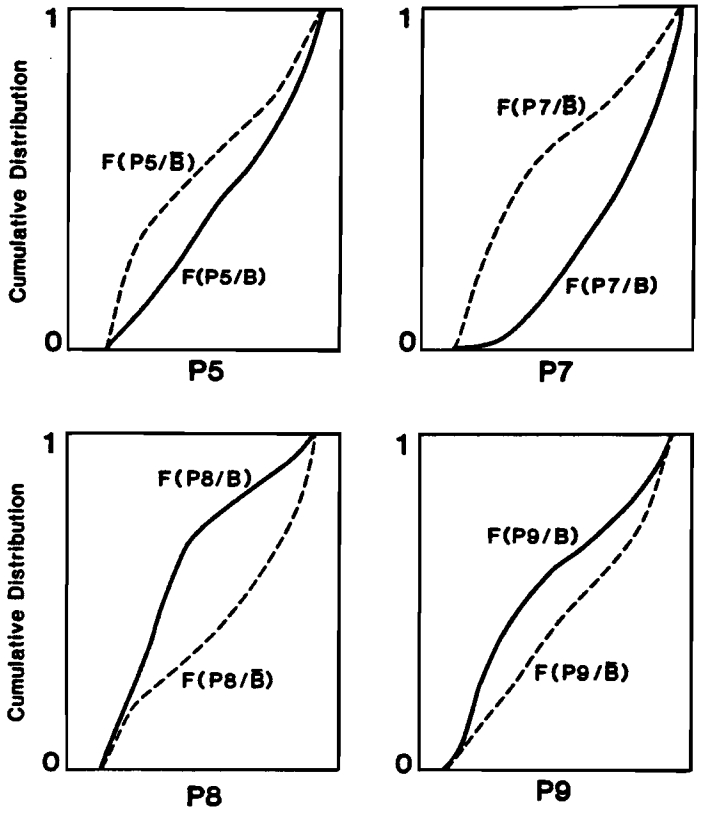

FIG. 2. Cumulative distributions of the four parameters in the hydrology model which significantly affected the value of the SSE criterion of model goodness of fit. The parameter distributions when the SSE was in the lowest 30% are indicated by $F(P/B)$; those when the SSE was in the highest 70% are indicated by $F(P/\bar{B})$.

up to 1.5 times the lowest SSE value obtained (Table 1). The parameter values corresponding to the "optimal" SSEs showed little consistency (Table 1). There appears to be a fairly large region of the parameter space from which "optimal" values can be chosen. These "optimal" values appear to represent local minima in a badly behaved SSE response surface.

A set of results similar to that for the SSE objective function was generated using the log likelihood function presented in [24]. The results were, of course, quantitatively different from those using the SSE, but the qualitative picture is very similar (Table 2). The response surface for the full model is evidently not improved by going from the SSE to the log likelihood criterion.

TABLE 1

PARAMETER VALUES FOR SSE OPTIMIZATIONS[a]

Run	Normalized Parameter													Relative SSE
	1	2	3	4	5*	6	7*	8*	9*	10	11	12	13	
1	0.0015	0.56	0.05	0.01	1.34	2.50	5.04	0.33	2.08	0.93	0.04	0.27	1.80	1.49
2	0.0015	0.08	0.67	0.02	1.07	0.23	0.89	0.52	1.43	0.82	1.00	1.91	0.81	1.27
3	1.26	0.22	0.001	0.92	1.15	0.84	4.42	1.25	0.27	0.95	0.01	1.36	0.14	1.16
4	0.23	0.0015	0.89	0.01	1.43	0.66	3.36	0.28	2.88	0.97	0.05	1.59	0.01	1.59
5	0.19	1.15	0.95	0.18	0.82	0.56	5.43	0.59	1.42	0.62	0.06	0.33	0.70	1.13
6	1.46	0.0010	0.97	0.01	0.97	0.55	8.03	0.33	1.44	0.50	0.12	0.002	0.80	1.35
7	0.0015	0.74	0.001	1.19	0.45	0.01	1.08	2.11	0.58	0.74	1.00	1.31	1.11	1.28
8	0.62	0.57	0.99	0.03	1.07	1.96	1.27	0.59	0.47	0.63	0.13	1.31	0.64	1.37
9	0.12	0.000	0.001	3.44	0.83	0.06	4.18	3.34	0.35	0.91	0.49	1.40	0.06	1.26
10	1	1	1	1	1	1	1	1	1	1	1	1	1	1

[a]On the full model, starting with random initial estimates. Parameter values are normalized to the values for the best run (run 10). Asterisks indicate the sensitive parameters as determined by the RSA procedure.

TABLE 2

PARAMETER VALUES FOR MAXIMUM LIKELIHOOD OPTIMIZATIONS[a]

	Normalized parameter													
Run	1	2	3	4	5*	6	7*	8*	9*	10	11	12	13	MLF[b]
1	0.03	89.11	0.02	0.44	0.83	0.43	4.48	1.39	0.67	0.86	0.94	0.07	1.33	1.11
2	24.26	88.93	1.12	5.37	0.71	0.14	1.46	7.49	0.13	1.04	0.53	0.05	3.58	5.25
3	2.26	16.68	0.17	0.03	1.29	0.96	0.69	1.21	0.30	0.64	0.92	7.82	3.64	5.08
4	0.03	85.36	0.02	0.68	0.29	0.03	0.61	9.19	0.08	0.86	0.002	1.23	0.16	1.05
5	2.21	2.07	0.52	0.01	0.93	4.13	0.71	0.38	1.23	0.68	0.64	0.77	0.01	1.21
6	0.03	4.20	10.70	3.41	1.03	1.34	1.63	0.86	0.27	0.71	0.01	1.38	0.87	1.13
7	11.32	85.71	0.02	0.01	0.76	0.06	0.87	0.38	0.85	1.15	0.96	0.01	3.04	1.49
8	7.66	0.88	0.02	9.10	0.92	0.32	2.72	8.97	0.05	1.04	1.00	0.73	5.21	5.05
9	0.03	3.21	2.45	3.97	0.82	1.20	0.29	2.47	0.32	0.80	0.00	0.69	3.83	1.68
10	1	1	1	1	1	1	1	1	1	1	1	1	1	1

[a] On the full model, starting with random initial estimates. Parameter values are normalized to the values for the best run (run 10). Asterisks indicate the sensitive parameter as determined by the RSA procedure.

[b] Relative maximum likelihood function.

TABLE 3

PARAMETER VALUES FOR SSE OPTIMIZATIONS[a]

Run	Normalized parameter				Relative SSE
	5	7	8	9	
1	1.05	1.26	0.98	0.71	1.01
2	1.05	1.23	0.98	0.71	1.01
3	0.96	0.79	1.02	1.35	1.03
4	0.94	0.81	4.42	1.45	1.20
5	0.45	0.17	2.11	3.64	2.98
6	1.00	0.97	1.00	1.00	1.00
7	1.05	1.20	0.98	0.72	1.01
8	1.00	0.96	1.00	1.01	1.00
9	1.00	0.99	1.00	1.00	1.00
10	1	1	1	1	1

[a]On the reduced model, starting with random initial estimates. Parameter values are normalized to the values for the best run (run 10).

We next examined the alternative of reducing the model structure by eliminating all processes in the model that were not identified as sensitive in the RSA. The resulting model, which still retains the topography-based structure of the original model, contains four parameters.

The SSEs for 10 optimizations of the four parameters from random starting points ranged up to 3 times that of the lowest value (Table 3). Even with the reduced model structure there are apparently local "depressions" in the response surface, some of which may be far from the global optimum. Most of the SSEs for the reduced model, however, are very close to the minimum value, and the parameter values associated with these are all within a few percent of each other (Table 3). Furthermore, even though the number of parameters has been reduced from 13 to 4, there is little loss in terms of the SSE criterion. The minimum SSE for the reduced model exceeds the minimum SSE for the full model by only 5%.

Sorooshian and Gupta [25] summarize much previous work that has addressed calibration of conceptual rainfall-runoff models and point out problems that have been noted. These include interdependence among model parameters, indifference of the objective function to certain parameters, discontinuities in the response surface, and nonuniqueness of the optimum values of parameters. It is clear from the results of both the regionalized sensitivity analysis and the optimizations that the objective function is, in fact, indifferent to all but a small number of the 13 model parameters in the full model and that the "optimum" value of the parameters is not well defined.

Sorooshian and Dracup [24] pointed out that in certain cases the shape of the response surface using a maximum likelihood function was much better than the SSE response surface. For calibration of our full hydrological model to WOR, this was not the case. The shapes of the response surfaces for the SSE and the maximum likelihood functions were very similar. No improvement in fitting the observed hydrograph using the full model was realized by employing the Sorooshian-Dracup method.

The use of the RSA to reduce the dimension of the parameter estimation problem appeared to work reasonably well in this case. The parameter estimates, with only a few exceptions, are stable in the sense that convergence was to approximately the same point in the parameter space. Thus, from the standpoint of the input-output data, there is little to recommend the full model over the reduced model, regardless of the fact that the processes that were included in the full model were inferred to be important from direct field observations.

EQUILIBRIUM CHEMISTRY MODEL

The hydrological model routes almost all precipitation through a single saturated zone store. Except during storm conditions, the water in WOR might therefore be considered to be in chemical equilibrium with a single (lumped) storage element. We have modeled the equilibrium chemistry of WOR using just such an assumption [6].

In applying the chemical model we again had a considerable quantity of data for WOR itself. Major ion chemistry has been analyzed on a weekly basis for WOR for several years [9]. On the other hand, data for soils and soil water (the store that presumably determines the chemistry) are sparse—certain data are available from isolated points in the catchment, but spatial coverage is necessarily limited and samples are usually not matched temporally with streamwater samples.

The questions that we address in this case are whether the model we propose is *consistent* with the sparse available data and, if so, whether we can identify the best measurements that might be made to test the model's adequacy using a quantitative (statistical) analysis. Because it is most natural to posit the behavioral criteria in terms of soil properties, we invert the "normal" calculation procedure and, using streamwater chemistry as "inputs," *compute* values of soil variables. (The "normal" procedure would be to compute streamwater chemistry from soil properties, since the water is presumed to flow from the soil to the stream.) The calculated soil variables are then the trajectories used in the behavioral classification.

In keeping with the lumped approach to modeling catchments, we postulated that a relatively small number of important soil processes—processes

that could be treated by reference to average soil properties—determine streamwater chemistry. In two papers, Reuss [19, 20] proposed a simple system of reactions describing the equilibrium between dissolved and adsorbed ions in the soil-soilwater system. Reuss and Johnson (in press) expanded this system of equations to include the effects of carbonic acid resulting from elevated CO_2 partial pressure in soils. Chemical conditions in the soil were assumed to be uniform throughout the depth being considered. Surface water chemistry was determined in the model by "removing" the soilwater from contact with the soil, allowing the excess CO_2 to degas to the atmosphere with subsequent precipitation of aluminum hydroxides as the solution pH increased.

We have extended this conceptual approach to include all of the important cations and anions present in WOR streamwater, and to include important complexation reactions involving dissolved aluminum. A total of twenty-four equations and five adjustable parameters describe the reactions that determine the chemical composition of soilwater in the model [6].

If the lumped equilibrium model is adequate and the parameters correctly chosen, the soil properties predicted by the model when driven with the observed streamwater chemistry should agree with actual measurements of the soil properties. Herein lie two problems:

(1) With which particular soil measurement should the model prediction at a given time be compared? Our measurements of soil properties are much less frequent in time than the stream measurements and additionally are spatially distributed.

(2) Are the parameter values used for the predictions consistent with the physical processes they are supposed to represent? The model is based on a lumped formulation, and the value chosen for a cation selectivity coefficient in the model, for example, may not be numerically equal to the experimentally determined cation exchange selectivity measured at some discrete point in the catchment.

Given the spatial heterogeneity of measured soil properties and little knowledge of the true values of the lumped model parameters, the question is best posed as what *ranges* of parameter values are most likely to produce model predictions of soil properties that are within the *ranges* of our distributed measurements of these properties. The adequacy of the model can then be judged in two ways. If we constrain the ranges of the parameters to some subset of possible values (e.g. based on literature values or a few field observations) and we are not able to reproduce the observed soil properties using parameter values chosen from these limited ranges, the model must be judged inadequate. Conversely, if we are able to reproduce the soil properties only by selecting parameter values that are unrealistic (e.g. solubility con-

stants that are clearly incompatible with the hypothesized solid phase of a substance in the model), the model again must be judged inadequate.

For this problem, then, the allowable ranges of selected soil properties form the basis of the behavioral classification. We chose four criteria for WOR. The first behavior criterion (B1) is that predicted base saturation of the soil, the percentage of exchange sites occupied by base cations (as opposed to aluminum), must be within the range that is realistic for the type of soil at WOR. The other three criteria (B2, B3, and B4) define ranges for acceptable values of soil–water pH, total dissolved aluminum, and the partial pressure of CO_2, respectively.

Values of five parameters must be selected in the model. Three of these (labeled P1, P2, and P3) are selectivity coefficients, coefficients which indicate the affinity of the soil exchange sites for cations of different valence. The fourth parameter (P4) is an aluminum solubility coefficient which indicates the extent to which the concentration of hydrogen ion in soilwater is buffered by the dissolution of an aluminum mineral. The last parameter (P5) specifies the fraction of sodium that is adsorbed on the soil.

Three hundred Monte-Carlo runs of the model were made and subsequently analyzed using the RSA procedure. Each of the five parameters showed sensitivity (as measured by the K-S statistic with $p = 0.01$) in at least one of the behavioral categories.

How might a particular set of parameter values, a set that would result in satisfactory simulation of *all* behavior criteria, be chosen? If such a set of values can be found, we will have, in a sense, "tentatively calibrated" the model inasmuch as we will have identified at least one scenario that was consistent with the sparse data available. We will have failed to reject this particular model structure on the basis of available information.

To determine a set a values for the parameters that would be consistent with available information, we adopted the *ad hoc* procedure described below. Under behavioral category B2, only the distribution of parameter P1 showed significant separation. This separation defined a value for acceptable results [Figure 3(a)]. Likewise, the distribution of parameter P5 showed a significant separation on behavior B4, allowing a value for P5 to be chosen [Figure 3(b)]. We selected values for these parameters as indicated in Figure 3.

The structure of the model is such that, by definition, behavior B1 is conditioned *only* by parameters, P1, P2, and P5. Having already chosen a value for P5, a contour plot of soil base saturation as a function of P1 and P2 can be constructed by running the model for different combinations of values of P1 and P2. The region of base saturation predictions that agrees with our field measurements determines an acceptable model behavior (Figure 4). Given that a value of P1 has also already been selected, a value of P2 can be

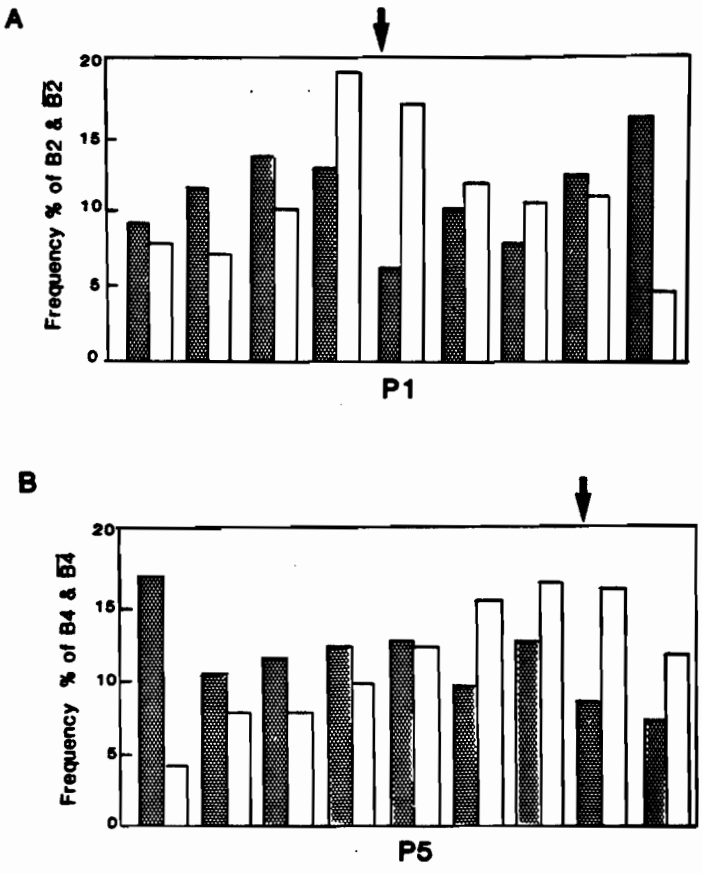

FIG. 3. Distributions of parameter values over their predefined ranges when the model produced acceptable behaviors (B, unshaded bars) and nonbehaviors ($\bar{B}$, shaded bars). The distributions are significantly different ($p = .01$) as determined by the Komolgorov-Smirnov statistic. (a) Parameter P1 and behavior criterion B2. (b) Parameter P5 and behavior criterion B4. In both cases, the arrows indicate the values of each parameter chosen as most likely to produce correct behavior and least likely to produce incorrect behavior.

chosen such that the point in the contour space of Figure 4 corresponding to the selected values P1 and P2 falls in the region of acceptable results. A value for P2 that maximizes the distance between this point and the boundaries of the acceptable region (intersecting lines in Figure 4) should give a high probability of the model producing acceptable values in terms of behavior B1.

Having selected values for P1, P2, and P5, we examined the two dimensional response surfaces of behaviors B2, B3, and B4 as functions of P3 and P4

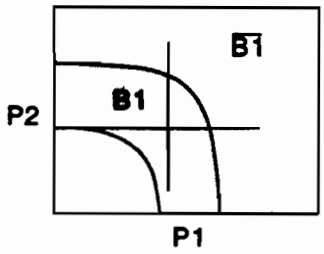

FIG. 4. A contour plot of model predictions of soil base saturation as a function of parameters P1 and P2. The enclosed region indicates the values of soil base saturation observed in the field. Model scenarios (choices of P1 and P2) that predicted base saturation in this region are classified as acceptable behaviors (B). Scenarios which predict base saturation outside this region are nonbehaviors ($\bar{B}$).

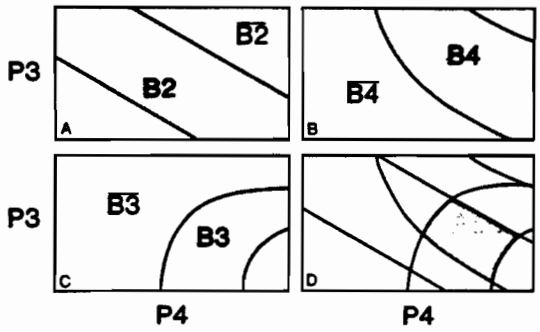

FIG. 5. Contour plots of (a) soilwater pH, (b) total dissolved aluminum in the soilwater, and (c) soil CO_2 partial pressure as functions of parameters P3 and P4. In each plot, the enclosed region indicates the values of the soil properties observed in the field. Model scenarios (choices of P3 and P4) that predicted soil properties that fell within these regions were classified as acceptable behaviors (B). The intersection of the regions in (a), (b), and (c) is indicated by the shaded region in (d). Choosing values of P3 and P4 in this region results in model scenarios for which all three behaviors (B2, B3, and B4) can be simultaneously obtained. A particular pair of values for P3 and P4 chosen by reference to the center of this region were considered to be most likely to result in all behaviors occurring simultaneously and were used for the final calibrated version of the model.

[Figure 5(a), (b), and (c)]. To complete the "calibration" of the model, specific values of P3 and P4 are selected such that behaviors B2, B3, and B4 are simultaneously obtained [Figure 5(d)]. The shaded area in Figure 5(d) is the intersection of the three behavioral regions indicated in (a), (b), and (c) respectively.

When the model is run with the values of the parameters selected according to the above procedure, the predicted properties for soilwater at

WOR are consistent with the available information. There are, obviously, any number of other combinations of values of the five parameters that would also be consistent. However, the model clearly points to certain soil properties and processes as being of critical importance in determining streamwater chemistry. Several of these, such as CO_2 partial pressure and cation selectivity, are not routinely measured in investigations of the role of acid deposition in soil and surface water acidification. If the conceptual basis of this model is correct, such information will be necessary in understanding the relationship between soil solution and streamwater chemistry.

DISCUSSION

Efforts aimed at the rigorous calibration and testing of complex models of environmental systems are often vitiated by the sparseness (or absence) of certain important data. In such cases a simpler model structure that is also compatible with available information may be devised. Often, however, a scientific study demands that certain structural aspects of the model be retained in that these pertain to the questions of importance to the study. The dilemma posed by Beck [2] intrudes: a small (rigorously calibrated) model may be all that the data can support in a statistical sense, given the premise of parsimony, but may be incapable of simulating certain physically interesting modes of behavior. On the other hand, a larger, complex model may produce behaviors that would never be observed in practice. In many problems in the environmental sciences the larger models are required, at least during certain phases of a study. We have presented a regionalized sensitivity analysis procedure that we maintain allows valuable inferences to be drawn in a speculative simulation modeling study.

The RSA procedure is more a heuristic than a rigorous statistical analysis. One of the more useful aspects of a study with the RSA is what might be called "hypothesis generation." By identifying the critical uncertainties in application of the model, one can argue that the RSA may lead to programs of study to reduce the uncertainties, i.e., to generate data to test critical hypotheses. This type of analysis was the motivation for the original development of the procedure [10, 26]. In the present study, the results have in fact led us to implement certain field studies. For example, the analysis of the equilibrium chemistry model led us to postulate that the production of CO_2 in the soil is extremely important in conditioning the streamwater chemistry in WOR and that the seasonal variability in this parameter should be pronounced, with CO_2 levels reaching a peak in September and a minimum in March. We have initiated a measurement program at WOR to test these ideas.

Another use of the RSA is as an objective means for reducing the dimensionality of a parameter estimation problem. Whitehead and Hornberger [30] showed that use of the RSA in this fashion led to the resolution of a problem of divergence when applying the extended Kalman filter to estimate the parameters in a mechanistic model of algal growth. Here we have shown that a hydrological model must be greatly reduced in complexity if stable parameters are to be obtained using only input-output data for WOR.

Perhaps the most important aspect of the regionalized sensitivity method is the ability to utilize nonstandard goodness-of-fit criteria. Because of the admissibility of nonanalytic and semiquantitative behavior criteria, we can deal with curve fitting in very broad terms and thus potentially develop insight into the system functioning that would not be readily gained in any other way. Auslander [1], in a study involving a complex, uncertain system, used the regionalized sensitivity method and concluded the following:

> The use of a statistically-based identification/sensitivity method is essential in such problems. ... A further observation, however, is that the type of information obtained from this technique gives a much stronger feeling for applicable parameter ranges than either identification procedures or sensitivity analyses based on point-by-point comparisons.

The fact that the RSA procedure worked to our satisfaction in this application to WOR cannot be taken as an indication that it will prove to be universally beneficial. The method proposed herein is not a well-defined and specific procedure for model identification and calibration, but rather an experimental approach that uses the computer as a "blunt instrument" as well as techniques of statistical inference. Nevertheless, it would appear that the general approach can be modified and elaborated to address a wide variety of practical problems.

Financial support for this work was provided by the National Science Foundation, the National Park Service, and the U.S. Environmental Protection Agency.

A portion of the work was accomplished while the authors were visiting the Department of Environmental Science, University of Lancaster, Lancaster, England. We gratefully acknowledge the support of Professor P. C. Young and his staff.

The research was funded in part by the EPA/NCSU Acid Precipitation Program (a cooperative agreement between the U.S. Environmental Protection Agency and North Carolina State University). It has not been subjected to EPA's required peer and policy review and therefore does not necessarily reflect the views of the Agency, and no official endorsement should be

inferred. This research has been funded as part of the National Acid Precipitation Assessment Program by the Environmental Protection Agency.

REFERENCES

1 D. M. Auslander, Spatial effects of the stability of a food-limited moth population, *J. Franklin Inst.*, submitted for publication.
2 M. B. Beck, Hard or soft environmental systems? *Ecol. Mod.* 11:233–251 (1981).
3 K. J. Beven and M. J. Kirkby, A physically-based variable contributing area model of basin hydrology, *Hydrol. Sci. Bull.* 24:43–69 (1979).
4 K. J. Beven and E. F. Wood, Catchment geomorphology and the dynamics of runoff contributing areas, *J. Hydrol.* 65:139–158 (1983).
5 R. T. Clarke, A review of some mathematical models in hydrology with observations on their calibration and use, *J. Hydrol.* 19:1–20 (1973).
6 B. J. Cosby, R. F. Wright, G. M. Hornberger, and J. N. Galloway, Modelling the effects of acid deposition: Assessment of a lumped-parameter model of soilwater and streamwater chemistry, *Water Resources Res.*, to appear.
7 K. Fedra, G. van Stratten, and M. B. Beck, Uncertainty and arbitrariness in ecosystems modeling: A lake modeling example, *Ecol. Mod.* 13:87–110 (1981).
8 K. Fedra, A Monte Carlo approach to estimation and prediction, in *Uncertainty and Forecasting of Water Quality* (M. B. Beck and G. van Stratten, Eds.), Springer, Berlin, 1983, pp. 259–291.
9 J. N. Galloway, G. M. Hornberger, and K. J. Beven, Shenandoah Watershed Acidification Study: Three year summary report, Nat. Park. Serv. Contract No. CX-001-9-0038, Dept. of Environ. Sci., Univ. of Virginia, Charlottesville, 1982.
10 G. M. Hornberger and R. C. Spear, Eutrophication in Peel Inlet I. Problem-defining behavior and a mathematical model for the phosphorus scenario, *Water Resources Res.* 14:29–42. (1980).
11 G. M. Hornberger and R. C. Spear, An approach to the preliminary analysis of environmental systems, *J. Environ. Mgmt.* 12:7–18 (1981).
12 G. M. Hornberger, K. J. Beven, B. J. Cosby, and D. E. Sappington, Shenandoah Watershed Study: A topography-based model of a small forested catchment. *Water Resources Res.*, submitted for publication.
13 R. B. Humphries, G. M. Hornberger, R. C. Spear, and A. J. McComb, Eutrophication in Peel Inlet III. A model for the nitrogen scenario and a retrospective look at the preliminary analysis, *Water. Resources Res.* 18:389–395 (1984).
14 R. P. Ibbitt and T. O'Donnell, Fitting methods for conceptual catchment models, *J. Hydrol. Div. Amer. Soc. Civil Engrs.* 97:1331–1342 (1971).
15 P. R. Johnston and D. H. Pilgrim, Parameter optimization for watershed models, *Water Resources Res.* 12:477–486 (1976).
16 G. Kuczera, On the relationship between the reliability of parameter estimates and hydrologic time series data used in calibration, *Water Resources Res.* 18:146–154 (1982).
17 R. G. Mein and B. M. Brown, Sensitivity of optimized parameters in watershed models, *Water Resources Res.* 14:229–303 (1978).

18 G. Pickup, Testing the efficiencies of algorithms and strategies for automatic calibration of rainfall-runoff models, *Hydrol. Sci. Bull.* 22:257–274 (1977).

19 J. O. Reuss, Simulation of soil nutrient losses resulting from rainfall acidity, *Ecol. Mod.* 11:15–38 (1980).

20 J. O. Reuss, Implications of the Ca-Al exchange system for the effect of acid precipitation on soils, *J. Environ. Qual.* 12:591–595 (1983).

21 J. O. Reuss and D. W. Johnson, Effect of soil processes on the acidification of water by acid deposition, *J. Environ. Qual.*, to appear.

22 H. H. Rosenbrock, An automatic method for finding the greatest or least value of a function, *Comput. J.* 3:175–184 (1960).

23 P. W. Shaffer and J. N. Galloway, Acid precipitation: The impact on two headwater streams in Shenandoah National Park, Virginia, in *International Symposium on Hydrometeorology*, Amer. Water Resources Assn., 1982, pp. 43–53.

24 S. Sorooshian and J. A. Dracup, Stochastic parameter estimation procedures for hydrologic rainfall-runoff models: Correlated and heteroscedastic error cases, *Water Resources Res.* 16:430–442 (1980).

25 S. Sorooshian and V. K. Gupta, Automatic calibration of conceptual rainfall-runoff models: The question of parameter observability and uniqueness, *Water Resources Res.* 19:260–268 (1983).

26 R. C. Spear and G. M. Hornberger, Eutrophication in Peel Inlet II. Identification of critical uncertainties via generalized sensitivity analysis, *Water Resources Res.* 14:43–49 (1980).

27 R. C. Spear and G. M. Hornberger, Control of DO level in a river under uncertainty, *Water Resources Res.* 19:1266–1270 (1983).

28 P. C. Young, The validity and credibility of models for badly defined systems, in *Uncertainty and Forecasting of Water Quality* (M. B. Beck and G. van Straten, Eds.), Springer, Berlin, 1983, pp. 69–98.

29 G. van Stratten, Analysis of model and parameter uncertainty in simple phytoplankton models for Lake Balaton, Tech. Rep. WP-80-139, Internat. Inst. for Appl. Syst. Anal., Laxenburg, Austria, 1980.

30 P. G. Whitehead and G. M. Hornberger, Modelling algal behaviour in the River Thames. *Water Res.* 18:945–953 (1984).

31 J. L. Vreeland, The role of shallow groundwater in the hydrogeochemical response of the White Oak Run catchment, Shenandoah National Park. M. Sc. Thesis, Dept. of Environ. Sci., Univ. of Virginia (1983).

32 T. R. Haelen, Hydrological and solution chemistry responses of a tributary valley in the White Oak Run catchment, Shenandoah National Park. M. Sc. Thesis, Dept. of Environ. Sci., Univ. of Virginia (1984).