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July 14, 2000
Contract No. NRC–02–97–009
Account No. 20.01402.762

U.S. Nuclear Regulatory Commission
ATTN: Mr. James Firth
Office of Nuclear Material Safety and Safeguards
Division of Waste Management
Performance Assessment and High-Level Waste Integration Branch
Mail Stop 7C–18
Washington, DC 20555

Subject: Transmittal of the Software Requirements Description for a Graphical Post-Processor for the TPA Version 4.0 Code (AI 01402.762.020)

Dear Mr. Firth:

The purpose of this letter is to transmit the Software Requirements Description (SRD) for the Total-system Performance Assessment Graphical Post-Processor (GPP), which fulfills the obligations of AI 01402.762.020. The SRD was prepared by Bayesian Systems, Inc. of Gaithersburg, Maryland, who are under contract to the Center for Nuclear Waste Regulatory Analyses to develop the GPP. Pending receipt of your approval of the SRD, we shall instruct Bayesian Systems, Inc. to prepare a Software Development Plan (SDP).

If you have any questions about the content of the SRD please call Dr. Osvaldo Pensado at (210) 522-6084.

Sincerely,

Gordon W. Wittmeyer, Ph.D.
Manager, Performance Assessment

GWW/jw
enc
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SOFTWARE REQUIREMENTS DESCRIPTION FOR A GRAPHICAL POST-PROCESSOR (GPP) FOR THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT (TPA) VERSION 4.0 CODE

Prepared for

Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

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July 2000

Gordon W. Wittmeyer 7/14/2000

Gordon W. Wittmeyer — Date
Performance Assessment

CONTENTS

FIGURES

1 INTRODUCTION

The purpose of the graphical post-processor (GPP) is to enable the user to develop, from the output of previously run Total-system Performance Assessment (TPA) code cases, graphical displays that will aid in the understanding and communication of the

- Repository performance
- Physical phenomena in the repository
- Effects of these phenomena on the performance
- Effects on performance of various possible modifications to repository design
- Degree of confidence/certainty about each of the above, based on the available evidence

Figures 1-1,1-2, and 1-3 illustrate the GPP output. Figure 1-1 shows the behavior of the key variables throughout the lifetime of the repository. See the glossary at the end of this document to clarify the meaning of relevant terms such as "variable." Taken as a whole, this figure displays the performance of the repository, and it has been, therefore, titled "Repository Performance Summary Diagram (RPSD)." The curves of figure 1-1 represent data aggregated from individual subareas, nuclides, or both.

Recognizing that there is uncertainty about this performance, stemming from uncertainty in modeling the physical phenomena and the future climate conditions, the software will quantify and communicate this uncertainty by displaying a set of RPSDs corresponding to different probability percentiles. For example, the user of the GPP could ask for a set of three RPSDs. One could show a median performance on each of the displayed variables. The second RPSD could show the 90th percentile performance for each of the displayed variables, and the third could show the 10th percentile performance. Note that showing, for example, the 90th percentile performance for multiple variables on the same page does not necessarily imply that such high performance in one variable is associated with high performance in another variable. The grouping of variables and percentiles on a graph is at the user's discretion.

This package of three diagrams would then quantify the state of knowledge of the repository's performance. Similarly, to explore a design change or a different assumption of future rainfall/climate conditions, one will use the GPP to prepare a new set of three (or more as needed) RPSDs to characterize the new performance. For example, figure 1-2 shows the infiltration before and after the construction of a subsurface diversion. The subsequent curves show the effect on the downstream variables before and after diversion.

The GPP will also assist in understanding various cause-effect relationships. For example, a correlation between the mean average temperature increase (MATI) at glacial maximum and the fraction of waste packages failed could be graphically depicted by a representation such as figure 1-3. Figure 1-3 displays a hypothetical positive correlation between the MATI variable and the fraction of waste packages failed.

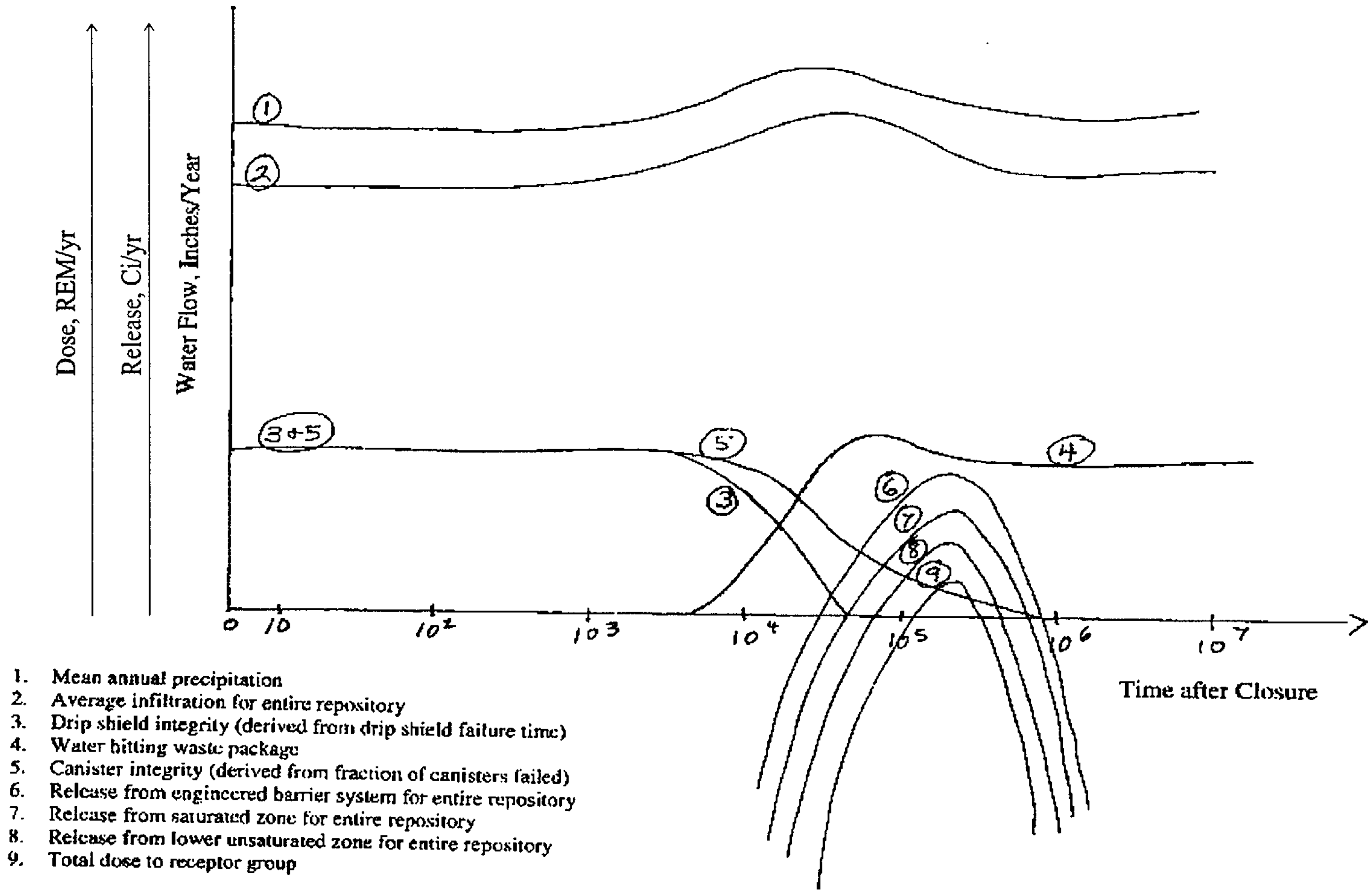
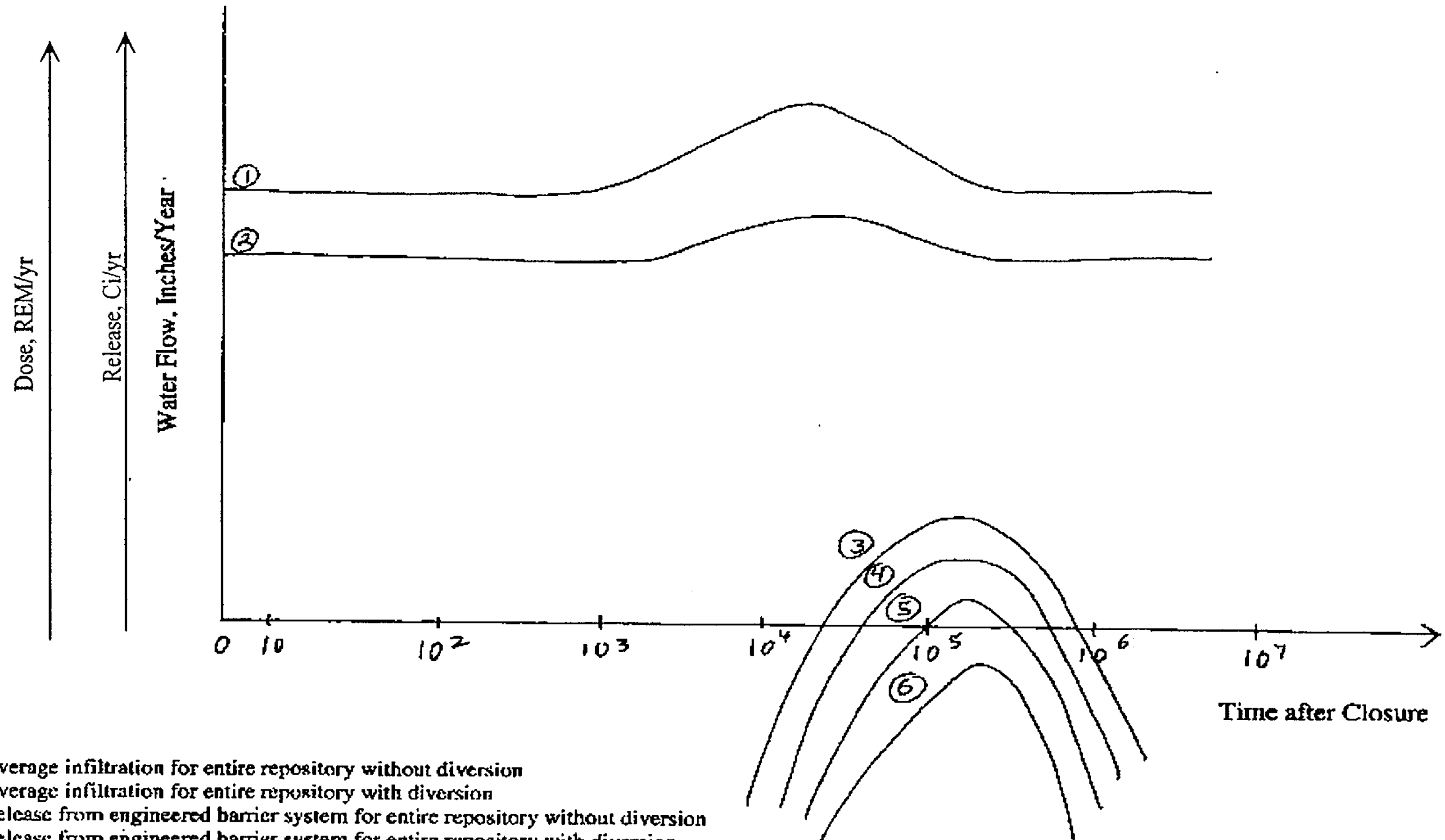


Figure 1-1. Repository performance summary diagram



1. Average infiltration for entire repository without diversion
2. Average infiltration for entire repository with diversion
3. Release from engineered barrier system for entire repository without diversion
4. Release from engineered barrier system for entire repository with diversion
5. Total dose to receptor group without diversion
6. Total dose to receptor group with diversion

Figure 1-2. Repository performance summary diagram: Effects of diversion strategy on water flow

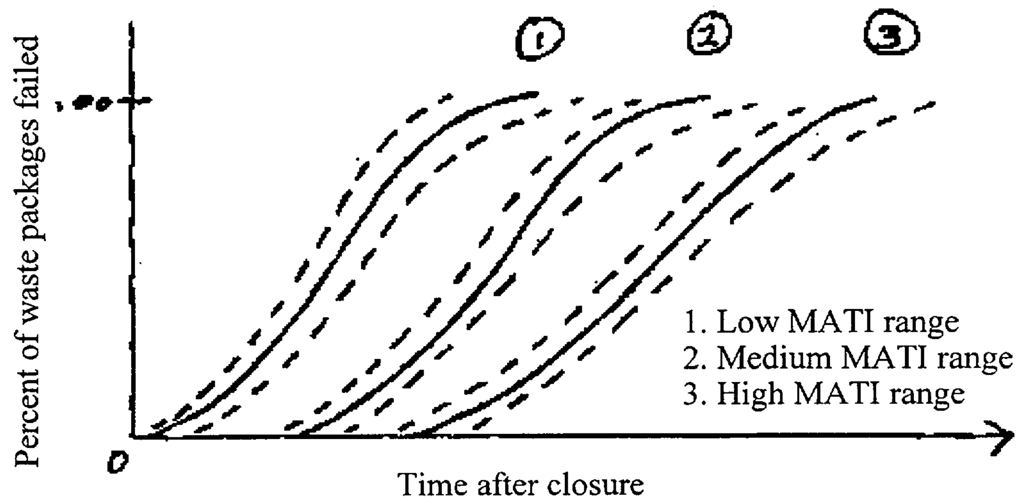


Figure 1-3. Effect of the mean average temperature increase (MATI) at glacial maximum on the percent of waste packages failed. Dotted lines represent uncertainty ranges.

2 SOFTWARE FUNCTION

The software will read TPA output files and graphically depict, for a selected repository configuration (i.e., a TPA code run), the time dependence on any of the following TPA variables

- Mean annual temperature
- Mean annual precipitation
- Infiltration per subarea
- Average infiltration per repository
- Average reflux per repository
- Average diversion per repository
- Fraction of canisters failed
- Drip shield failure time
- Water hitting waste package
- Repository temperature
- Waste package temperature
- Waste package relative humidity
- Release from engineered barrier system per subarea
- Release from engineered barrier system per repository
- Release from lower unsaturated zone per subarea
- Release from lower unsaturated zone per repository
- Release from saturated zone per subarea
- Release from saturated zone per repository
- Current biosphere dose conversion factors
- Pluvial biosphere dose conversion factors

- Total dose to the receptor group
- Peak dose for compliance period

The software will be able to plot for any set of realizations and any of the mentioned variables, either (i) the bundle of trajectories showing for each realization the value of the variable during time, (ii) a single curve summarizing the bundle by representing the median (50th percentile) value of the variable for each time, or (iii) a family of curves containing not only the median curve described previously, but also the curve for any other percentile. The TPA code allows many input parameters to be expressed as a probability distributions that vary over some ranges. The family of curves portrays not only the median trajectory for the variable, but also the combined effect of such variation in input parameters. Such a family of curves enables visualization of the confidence intervals associated with any curve.

The software will graphically depict the degree to which any given TPA input parameter or output variable affects a TPA output variable by

- Enabling the user to select for any TPA output variable, a parameter or variable whose influence the user wants to explore

- Partitioning any set of realizations into subsets based on the range of values for the parameter or variable, and plotting for each subset either the median curve or the family of percentile curves

- As a special case of the previous bulleted item, for any TPA input parameter specified as a distribution, enabling the user to restrict the range of values for that parameter. Such a restriction results in pruning the set of realizations from which the curves are calculated and, therefore, enables the user to visualize the degree to which TPA output may be controlled by any given TPA input parameter.

The capabilities described in the previous paragraph allow the user to ask a wide variety of "what-if" questions concerning how the repository will respond during various interventions or design options. For example, one family may represent the realizations with a high waste package temperature, while another may represent the realizations with a low chloride concentration.

The software will be able to account for the values of any variable, calculated by the TPA code on a per subarea or per nuclide basis.

3 COMPUTATIONAL APPROACH

Standard object oriented design will be employed.

Standard Java coding conventions will be employed.

Custom code will be minimized.

The software will enable the user to
- Control the windows in which plots are displayed

- Control for any plot the appearance of the following visual components
  - Background color
  - Box
  - Legend
  - Title

- Control for any axes of a plot
  - What is the range and kind of scale (linear or logarithmic) used
  - How the axis is labeled
  - What color is used or what variable is mapped to the color
  - What range of values to include
  - Which field is mapped to that axis

- "Snap" or capture, from any plot currently open, an image file that may be stored in "JPEG" or "PNG" format

- Write values for any data being plotted to a disk file in a tabular format

- Select parameters or variables whose influence on the displayed variable the user wants to explore

- Perform side-by-side visual comparisons of different plots

4 TECHNICAL BASIS: PHYSICAL AND MATHEMATICAL MODEL

The TPA GPP is the response to the Advisory Committee for Nuclear Waste (ACNW) suggestion to develop a way to visualize and understand the performance of the repository and the effect of various assumptions and design changes on that performance. Figures 1-1 and 1-2 are examples of the type of graphical output that the GPP will produce.

Figure 1-1 graphically summarizes the overall performance of the repository and the physical phenomena in it. This figure recognizes that the movement of water is the key phenomenon (without which there would be no release of radioactivity). Thus, curve 1 presents the surface rainfall as a function of time. Curve 2 shows infiltration (which could be different from curve 1 if surface drainage were provided). Curve 3 indicates canister integrity and curve 4, drip shield integrity. Curve 5 shows water hitting the waste package. Curve 6 states the release from the engineered barrier system. Curve 7 presents the release from the lower unsaturated zones and curve 8, the release from the saturated zone. Curve 9 indicates the total dose. Ultimately the canister degrades leading to transport of radioactivity to the unsaturated and saturated zones, the biosphere, and the target group.

Figure 1-2 reflects how the performance of the repository would change if a subsurface diversion path were provided. These and similar figures could give understanding of the elements determining repository performance and suggest how that performance could be improved by various interventions or design options. Such a repository change could be simulated by the TPA code by a change in the mean annual infiltration.

GLOSSARY

Throughout this document *variable* represents one of the quantities that a user will want to plot and that is often a function of time.

Parameter refers to the values (specified in file tpa.inp) that affect the variables in TPA realizations.

A *partition* for set S is a collection of disjoint subsets of S such that every element of S is in exactly one of the subsets.

A *trajectory* refers to the projected time history for one variable. This is a curve or scalar function of time.