MODIFICATIONS TO DITTY COMPUTER CODE AND ITS LINKAGE TO THE TOTAL SYSTEM PERFORMANCE ASSESSMENT CODE

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INTRODUCTION

A version of the DITTY (Dose In Ten Thousand Years) code was received by the Center for Nuclear Waste Regulatory Analyses (the Center) in the summer of 1991. It was decided through discussions among team members that DITTY will be used as the dose calculation module in Iterative Performance Assessment (IPA) Phase 2. Minor modifications were made to DITTY in the process of linking it to the Total system Performance Assessment (TPA) code. The modifications made, as well as the various links established between DITTY and TPA, are briefly described in the following.

The DITTY computer code was originally developed at the Battelle Pacific Northwest Laboratory specifically for application to high-level waste isolation primarily at the Hanford site. This code estimates the time integral of collective dose over a ten thousand year period for time varying radionuclide releases to the environment which includes surface waters (rivers and lakes), ground waters (wells), and the atmosphere. In the original code, the time frame for the calculation of dose is 10,000 years. This 10,000 year time span is subdivided into 143 periods, each of 70 year duration - 70 years being the average human-life span in which the dose is assumed to be received. The average radionuclide release to the environment in each of these 70 year periods is assumed to be provided as input to the dose code. From this, the population dose is determined for each period. The total radioactive material present during any period is taken as the sum of material released during that period and residual material in the environment from release in previous periods. The original program is designed to run in a stand-alone mode with no other controlling process except the host operating system. Modifications described below were made to adapt the DITTY code so that it would run under the commands of the TPA code.

DESCRIPTION OF MODIFICATIONS TO DITTY

In the Total system Performance Assessment, DITTY will be one of many "consequence modules" that would be executed in a specified sequence. Thus, to be useful as part of the TPA code, DITTY must be able to interact with the TPA - the executive program. This was the primary objective for the modification of DITTY. A few other changes were also made for convenience as detailed below. Modifications are numbered sequentially in the following, for ease of reference and discussion.

The original DITTY code was designed to perform dose calculations for 10,000 years in 143 life spans of 70 years each. To introduce some flexibility, the following modifications were made.

1. A parameter MAXPER (denoting maximum number of periods) is defined to replace the number 143. All arrays whose dimension depend upon the number of 70 year periods used in the calculations are now dimensioned by using the parameter MAXPER. Thus by changing the value of MAXPER, the code can now be compiled to fit calculations for any number of periods. The default value of MAXPER is currently set to 1430 which corresponds to a calculation period of 100,000 years.

2. A new variable MAXT (denoting maximum time for calculations) is introduced where MAXT is the number of years for which calculations are to be performed. It replaces the number 10,000 years in the original code. MAXT is used to check when to stop the calculations. Thus the code can now be used to perform dose calculations for any desired time span. The current default value of MAXT is 10,000 years. As will be explained in the following, the value of MAXT can be provided from the TPA code. Note that while MAXPER is a dimensioning parameter, the variable MAXT is used to decide when to stop calculations.

The length of the life span (i.e., 70 years) is still fixed in the code. In future, this should also be changed by a variable so that it can be modified by the user. However such a modification is expected to be quite involved.

3. A subroutine RDDAT has been created to read the global data file. The global data file contains run parameters which are pertinent to a particular scenario, and which are common to one or more consequence modules. This file may contain the times at which calculations for a particular scenario are to begin and end. This file may also contain the names of the radionuclides that are to be used in calculations. Note that most consequence modules are required to receive some of their data from the global data file. As an interface between a consequence module and the TPA, a subroutine must be added to read such data and place it in appropriate arrays. Unfortunately, we have not yet found a better way for doing this and hence a subroutine must be designed for each consequence module. RDDAT is such a subroutine for DITTY. The time to end the simulations provided to DITTY in the global data file is provided through the variable MAXT described above.

4. A subroutine RDMAP has been added. This subroutine reads data from the Latin Hypercube Sampling (LHS) output file. The map file contains a correspondence (or map) table that tells the DITTY code the locations in the LHS output file where quantities needed by the DITTY code are stored. Note that the DITTY code is designed to function as a deterministic code in its normal mode. However, the TPA code is designed to perform in a Monte Carlo mode for each scenario. All of the statistically defined parameters are sampled once by the LHS module at the beginning and the sampled values are written to a file. Each consequence module then reads the sampled values pertaining to it from this file. Again, we do not yet have an automatic way of passing this information except through a subroutine like RDMAP. Note that for RDMAP (also RDDAT) to work, the user has to make *a priori* (before compiling) decisions as to which parameters are to be sampled.

5. A provision has been added to write a special output file to transfer the calculated dose data to the system code. The system code processes this data to calculate the Complementary Cumulative Distribution Function (CCDF) of dose for either a single scenario or for all scenarios combined.

6. Another feature added to DITTY is the generation of a TECPLOT file for generating a time versus dose plot. TECPLOT is a commercial product available for personal computers and the Silicon Graphics workstation, which facilitates interactive plotting of formatted data files.

7. Subroutine MAKDA2 was modified to accommodate access to the host operating system date and time functions. The date and time functions are used to time stamp the output for run identification. It may be better to affect this by using the preprocessing preFOR utility developed at the Center, but that has not been done yet.

8. Subroutine OPNFIL was modified to open the global and map data files when DITTY is used as a consequence module with the TPA system.

9. To provide an easy mechanism for data entry, the input variables were changed to NAMELIST members. This allows the name of the variable to be specified with the data value associated with it. The input is then more readable and variables absent from the input file are assigned default values.

10. The DITTY program was originally written to allow many cases to be analyzed in one run. This feature was changed to a one case per run mode which will allow the system code to collect and store any intermediate data for CCDF calculations before proceeding to the next vector run.

SUMMARY AND CONCLUSIONS

The PNL dose code DITTY has been adapted for use in IPA Phase 2. This involved making some modifications which included defining one new parameter and one variable. In addition, two subroutines were added to provide the interface with the TPA code. Minor modifications in a few of the existing subroutines were also made.

In the future, for IPA Phase 3, the DITTY code may be further modified to: (1) Use the preFOR utility so that system calls such as for obtaining run time and date for different machines can be automated; (2) Modify the code so that the length of the calculational period can be different from 70 years; and (3) Study in greater detail the mechanistic calculation algorithms in DITTY and replace some of them with more updated ones. One such algorithm may be the one that deals with atmospheric dispersion or organ weighting factors.