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Qualification Plan for the Genmod-PC Computer Program

Plan d'homologation pour le programme informatique Genmod-PC

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July 2002 juillet

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RÉSUMÉ

Genmod-PC est un code dosimétrique exécutable sur le système d'exploitation Windows qui permet de calculer les doses et apports de radionucléides pour un adulte du sexe masculin. Le plan d'homologation contenu dans le présent rapport vise à déterminer les facteurs d'assurance qualité conformément aux recommandations de l'Association canadienne de normalisation et aux modalités d'application en ce qui a trait à un programme informatique existant élaboré par EACL.

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ABSTRACT

Genmod-PC is an internal dosimetry code that uses the Microsoft Windows® operating system, and that currently calculates radionuclide doses and intakes for an adult male. This report provides a plan for specifying the quality assurance measures that conform to the recommendations of the Canadian Standards Association, as well as AECL procedural requirements for a legacy computer program developed at AECL.

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1. INTRODUCTION

1.1 Objective

Atomic Energy of Canada Limited (AECL) is committed to satisfying the requirements of Canadian Standards Association (CSA) Standard N286.7-99 [1] for all analytical, scientific and design computer programs developed, purchased and used by AECL. To this end, AECL has developed a quality assurance manual (QAM) for analytical, scientific and design computer programs [2]. The QAM stipulates that a legacy computer program, such as Genmod-PC, must undergo a qualification process before it can be used in new safety analysis studies.

The procedures that specify the qualification (verification) requirements of a legacy computer program developed at AECL are defined in AECL Procedures 00-561.1 [3] and 00-451.1 [4]. This qualification plan is prepared in accordance with AECL Procedure 00-461.3 [5]. The Genmod-PC qualification plan outlined in this document conforms to these requirements.

1.2 Genmod-PC Background

The Genmod internal dosimetry code (Table 1) has been an ongoing project since 1979 [6]. Recommendations for upgrading the internal dosimetry code Genmod were prepared in 1994 [7]. In 1996, work began on Genmod-PC for Microsoft Windows® using the C++ programming language and its object oriented features [8]. Genmod-PC, which uses Windows, currently calculates doses for an adult male [9]. The International Commission on Radiological Protection (ICRP) publication no. 66 [10] respiratory tract model, and the ICRP 60 [11] radiation and tissue weighting factors and dose calculation methodology are implemented. The code utilises specific effective energy (SEE) values from the SEECAL code written by Cristy and Eckerman [12]. Currently, there are ICRP models for the radionuclides of 29 elements in Genmod-PC for Windows, including models for the ^{3}H and ^{14}C compounds.

A documentation and verification control program was established with the Genmod-PC V3.0 (DOS version) release. Starting with pre-design planning of the Windows version of the code (and continuing throughout the development program), the developers of Genmod-PC incorporated quality assurance measures that followed the recommendations of the draft CSA Standard N286.7 (1992) [7, 13]. This quality assurance process generated extensive documentation in both protected AECL/COG reports and in refereed publications in the open literature, as described in Section 1.3.1 of this qualification plan. As part of the quality assurance of the code, validation by peers or "beta testing" was also carried out. Copies of the code, especially from 1998 onwards, were made available for beta testing to international organisations and experts in internal dosimetry. The beta testers sent back comments to the developers of Genmod-PC, and changes to the code were made to improve the code in terms of reducing errors, improving data displays, and improving user friendliness.

Table 1. Revision history of the Genmod-PC code and technical manuals [14-17].

Revision	Date	Comment
0.	1998 March	Original release with version 4.9 of the software.
1.	1999 March	Upgrade release with version 4.12 of the software. Additional models (Pu, Am, Np, Cm, alkaline earths, I, Fe, ^{3}H, C). Upgrades to configuration set-ups, SEE (U), intake estimate routines and the addition of secondary derived quantities output.
2.	1999 September	Upgrade release with version 4.14 of the software.
3.	2000 January	Additional model (C (methane)). Upgrade release with version 4.17 of the software.
4.	2000 April	PAS processing, multi-case mode. Upgrade release with version 4.19 of the software.

1.3 Current Conditions

The QAM declares that a computer program developed prior to the promulgation of CSA Standard N286.7-99 [1] must be verified if it is used for significant new analysis. The development of Genmod-PC predated this event and must therefore undergo the qualification process as outlined in the QAM. The qualification process specified by the QAM requires verification for the theoretical background, the software requirements specifications, the design descriptions and the coding.

1.3.1 Genmod-PC Compliance with AECL Software QA Manual

Most of the formal documents that are required for the QA process [5] were produced during the development of the Genmod-PC code:

1. The program abstract is effectively given in COG report COG-93-476, entitled "Recommendations for the Upgrade of the Internal Dosimetry Code, Genmod", written by Richardson [7].

2. The theory manual is effectively given in COG report COG-98-105, entitled "Genmod-PC - Technical Reference Manual", written by Richardson and Dunford, 1998-2000 and Richardson et al. 2000 [16, 17]. This manual has undergone five revisions (Table 1). The coding, incorporation, and verification and validation of the ICRP 66 respiratory tract model into Genmod-PC were documented as a master's degree thesis by Corns in 1996 [18]. Implementation of the dosimetry for compounds of tritium and ^{14}C was particularly difficult; Richardson and Dunford [19] describe the models in full in a refereed journal publication.

3. The user's manual is given in COG report COG-98-106, entitled "Genmod-PC – User's Guide", written by Richardson and Dunford, 1998-2000 and Richardson et al. 2000 [14, 15]. This manual has undergone five revisions (see Table 1).

4. The validation report is the major part of the work that is needed to demonstrate compliance, although some aspects of this report are to be found in the "Genmod-PC - Technical Reference Manual" [16, 17].

5. A version tracking report is required, although some aspects of this report are to be found in the "Genmod-PC - Technical Reference Manual" [16, 17].

2. GENMOD-PC QUALIFICATION PROCESS

2.1 Application Documentation

AECL Procedure 00-461.3 requires the following application documentation for legacy programs that are to be qualified: computer program abstract, theory manual, user's manual, validation report, and version tracking record.

As described in the section 1.3.1, much of the material for the requirements has already been written.

2.2 Validation and Verification

Analytical errors and conditions under which the computer crashes have been noted during the use of Genmod-PC v4.19 over more than two years. In particular, run errors were identified during current initial investigations into defining the appropriate verification exercises that should comprise a comprehensive validation and verification of Genmod-PC. After code changes have been made to eliminate these errors, the validation and verification of the new version, i.e., Genmod-PC v4.20, will begin in earnest.

The order of proposed verification exercises is listed in Table 2. An objective of this first formal quality assurance of the Genmod-PC code is to automate the process as much as possible to allow the process to be easily repeated for change control. This objective is important, as the ICRP continually publishes ICRP publications that recommend new methods to carry out internal dosimetry, e.g., changing from the ICRP's current simple gastrointestinal model [20] to a more complex gut model in the future. Funding proposals are also under review or envisaged, that will extend the range of individuals and radionuclide intakes for which the dosimetry can be assessed using Genmod-PC. For example, calculation of doses for adult males only will be extended to infants and children. The qualification report will be written as the verification exercise data are collected. The last task in the validation and verification exercises will be the finalisation of the various documents listed in Section 2.1 above.

Table 2. Proposed Verification Exercises

Exercise #	Validation and Verification Exercises	Runs Manual or Automated	Approx. number of runs (**E**, **I** see below)[a]
0.	**Correction of Mistakes Known to Users**		
	0.1 Compilation of bugs and other changes required.		
	0.2 Code modified and a new version v4.20 produced.		
	0.3 Code run and results verified to confirm that changes made have desired effect.		Exercise 2 repeated >20 times
1.	**Validation of Numerical Parameters for Each Element**		
	Values in Genmod compared with reference parameter values that are found in ICRP publications, unless stated. 1.1 Run Genmod and check, for each element, the model parameters displayed on the editing screen. 1.2 Check the data input file, Genmod.ini, for all elemental models, e.g., references, lung depositions, gut absorption factors, urinary-to-fecal ratio, compartment fractions and rate constants, etc. 1.3 Visually check that the biokinetic model equations given in the elemental C++ file (e.g., I-Elemental.cpp) match the latest ICRP publication's description of the model. 1.4 Visually check examples of specific effective energy values with source values by Cristy and Eckerman [12].	**M**	30 (**E**)
2.	**Validation of Dose Coefficients, Bioassay and Intake Activities**		
	2.1Equivalent and effectives doses compared to ICRP CD ROM [21] for the following cases: (*i*) F, M, S particle solubility, 1- and 5-μm particle size for each, and (*ii*) ingestion.	**A**: Each radio-nuclide and compound	70(**I**)·(3+1)·2 = 560
	2.2 Bioassay activities and concentrations compared to ICRP 78 [22] (other reference data being sought) for the following cases, where appropriate: (*i*) lungs, (*ii*) whole body, (*iii*) urine concentration, (*iv*) fecal concentration, and (*v*) organ (e.g., thyroid).	**A**: Selected radio-nuclide	70(**I**)·(3+1)·2 = 560
	2.3 Genmod-PC intake activity generated when using ICRP 78 [22] data (other reference data being sought) for **one** of the following bioassay cases: (*i*) lungs, (*ii*) whole body, (*iii*) urine concentration, (*iv*) fecal concentration, or (*v*) organ (e.g., thyroid).	**A**: Selected radio-nuclide	70(**I**)·(3+1)·2·4 = 2240

	2.4 Genmod-PC intake activity generated when using ICRP 78 [22] data (other reference data being sought) for **two or more** of the following bioassay cases: (*i*) lungs, (*ii*) whole body, (*iii*) urine concentration, (*iv*) fecal concentration, or (*v*) organ (e.g., thyroid).	**A:** Selected radio-nuclide	70(**I**)·(3+1)·2·4 = 2240
3.	**Validation of ICRP 66 Lung Model and Gut Model**		
	3.1 Visually check lung numerical parameters shown on editing screen against ICRP 66 [10], and gut model parameters against ICRP 30 [23].	**M**	
	3.2 Visually check that the lung and gut biokinetic model equations given in elemental C++ files match those of ICRP 66 [10] and ICRP 30 [23], respectively	**M**	
	3.3 Compare lung region depositions, clearances, etc. to ICRP 66 [10] or LUDEP [24], varying (*i*) particle size, (*ii*) density, and (*iii*) shape factor.	**M**	30
4.	**Verification of Menus, Graphics and File Handling**		
	4.1 Utilise each menu item.	**M**	50
	4.2 Graphics output (check values generated in 2(*b*) above).	**M**	5
	4.3 Output and file handling.	**M**	10
5.	**Debug Execution and Document**		
6.	**Summarise Findings**		
7.	**Validation of Results**		
	7.1 Identify and log the results of benchmark (reference) cases for dose assessments.		
	7.2 Check the results of non-default lung model parameter changes against LUDEP [24].		
	7.3 Log the results of non-default gut model parameter changes.		
	7.4 Log the results of non-default organ model parameter changes.		
	7.5 Identify and log the results of bioassay benchmark (reference) cases for various bioassay assessments and intake estimate methods.		
8.	**Theory Manual**		
9.	**User's Manual**		
10.	**Qualification Report**		

[a] Number of elements E = 30; number of isotopes and compound models I = 70.

2.3 Non-Conformances

i. The present computing environment for Genmod-PC is an unsupported Borland development system. This environment will not be changed before the validation and verification proposed here takes place. The justification for this is that the methods and documentation enacted for the current quality assurance program will make this process far easier when carried out the second (and subsequent) time(s) after the operating environment and other changes are made.

ii. The dosimetry for the elemental model for radon is currently calculated in the same manner as other elements. Namely, radon progeny are deemed to act biokinetically as their parent radionuclide. At a later date, the elemental model for radon will be modified so that it conforms to the ICRP recommendations, which recommend that each radon progeny be treated by their respective elemental model.

iii. The method employed to calculate the urine interval (Bq) and fecal interval (Bq) is currently incorrect. This method will be corrected in a later version of the code.

iv. There are uranium models in Genmod-PC for depleted uranium, high and low enriched uranium, and natural uranium. The option will be given in a later version of Genmod to display and print out values for the percentage mix of uranium isotopes; also, the user will be able to change the isotopic mix.

3. SCHEDULE

This verification and validation of Genmod-PC is described in the AECL intranet file called "rdplan", under the project entitled, "Complete and issue qualification plan for GENMOD computer program for internal dose calculations". Funding has been approved and work commenced on the first two tasks given below. The work project number is CV-220033.

Low-task #1. Prepare a work plan, including an outline of the qualification plan. Commence verification of execution runs. Start 2002 April 1, finish 2002 September 30.

Low-task #2. Tabulate data from verification of execution runs. Prepare draft documentation for this verification. Start 2002 October 1, finish 2003 March 31.

Low-task #3. Validate the results of the code and prepare a draft report. Start 2003 April 1, finish 2004 March 31.

Low-task #4. Finalise the validation and verification documentation. Start 2004 April 1, finish 2004 September 30.

4. CONCLUSIONS

This report has outlined a plan for the qualification of Genmod-PC. The plan complies with standards defined in the QAM. The plan describes the application documentation that will be produced. Much of the material required in the documentation has been published previously as COG reports. This material will be upgraded to comply with the requirements. The major effort needed to demonstrate compliance will be in providing a validation report.

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