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heheehA COMPUTATIONAL CODE FOR RESOLUTION OF GENERAL COMPARTMENT MODELS APPLIED TO INTERNAL DOSIMETRY

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ABSTRACT

The dose resulting from internal contamination can be estimated with the use of biokinetic models combined with experimental results obtained from bioanalysis and the knowledge of the incorporation time. The biokinetics models can be represented by a set of compartments expressing the transportation, retention and elimination of radionuclides from the body. The ICRP publications, number 66, 78 and 100, present compartmental models for the respiratory tract, gastrointestinal tract and for systemic distribution for an array of radionuclides of interest for the radiological protection. The objective of this work is to develop a computational code for designing, visualization and resolution of compartmental models of any nature. There are available four different techniques for the resolution of system of differential equations, including semi-analytical and numerical methods. The software was developed in C# programming, using a Microsoft Access database and XML standards for file exchange with other applications. Compartmental models for uranium, thorium and iodine radionuclides were generated for the validation of the CBT software. The models were subsequently solved by SSID software and the results compared with the values published in the issue 78 of ICRP. In all cases the system is in accordance with the values published by ICRP.

1. INTRODUCTION

The Nuclear and Energy Research Institute (IPEN/CNEN-SP) run facilities where radioactive materials are handled during the radiopharmaceuticals and fuel element production. Some of these activities involve the handling of unsealed sources, presenting risk of incorporation by the worker. To estimate the resulting doses of such activities, the Office for Radiation Protection has established an internal monitoring program based on air contamination analysis and the in vivo and in vitro measurement techniques.

The determination of the intake of a radionuclide by a worker involves the results of measurements, the use of biokinetic models, the knowledge of physical and chemical characteristics of the contaminants and also the moment when the incorporation has occurred.

The International Commission on Radiological Protection (ICRP) regularly publishes biokinetic models that describe the behavior of some radionuclides in the human body [1].. These models have been revised, allowing a more realistic description of the processes of absorption, retention and excretion of the incorporated material.

Several computer codes have been developed in order to support the internal dose calculation. They are based on the resolution of the system of differential equations that arises from the representation of biokinetic models for a set of compartments. This resolution can be obtained by analytical or numerical methods or even combining both.

The aim of this paper is to present the computer system developed at IPEN to be used during the internal dose estimation. The program developed allows the construction, visualization and resolution of biokinetic models by different mathematical techniques.

2. SYSTEM ARCHITECTURE

According to the internal dosimetry group requirements, it was defined a system architecture consisting of two independent programs. This architecture is schematically represented in Figure 1.

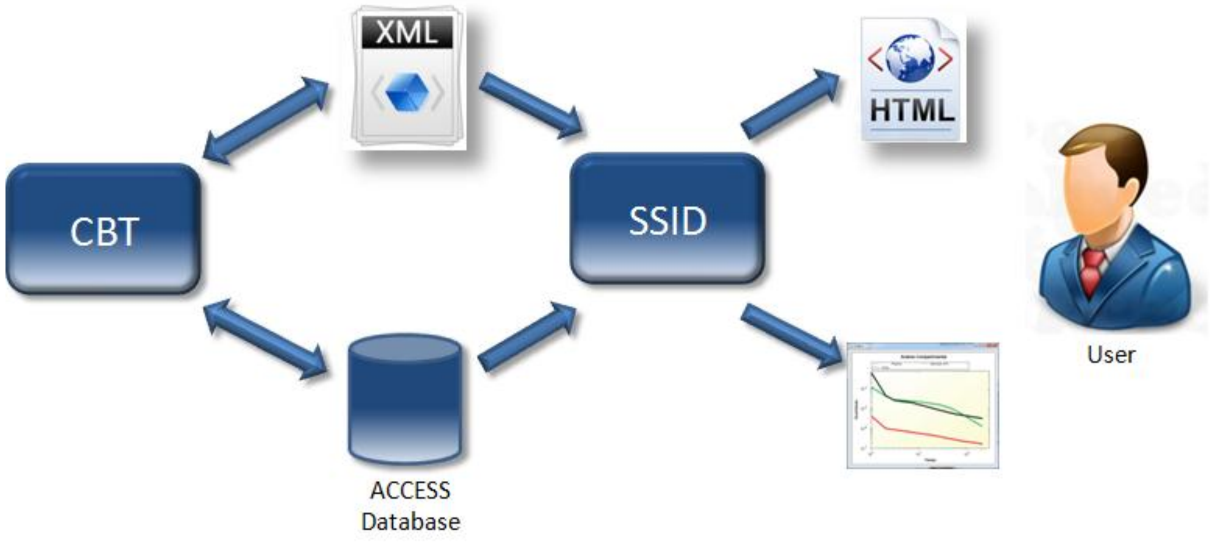


Figure 1. Architecture of the developed system.

The module called CBT (Compartment Builder Tool) is responsible for writing and reading information on the models, both in the database created in Access and in XML (eXtensible Markup Language), a markup language that defines a standard for exchanging information between applications written in different languages.

The module referred to as SSID (Smart Software for Internal Dosimetry) reads these models, assembles a system of differential equations, solve the equations using a mathematical method and present outputs as a data table and a graph.

The program was written in C# programming language, an object-oriented language, released by Microsoft in 2002 to be part of the programming languages that compose the .NET development platform [2].

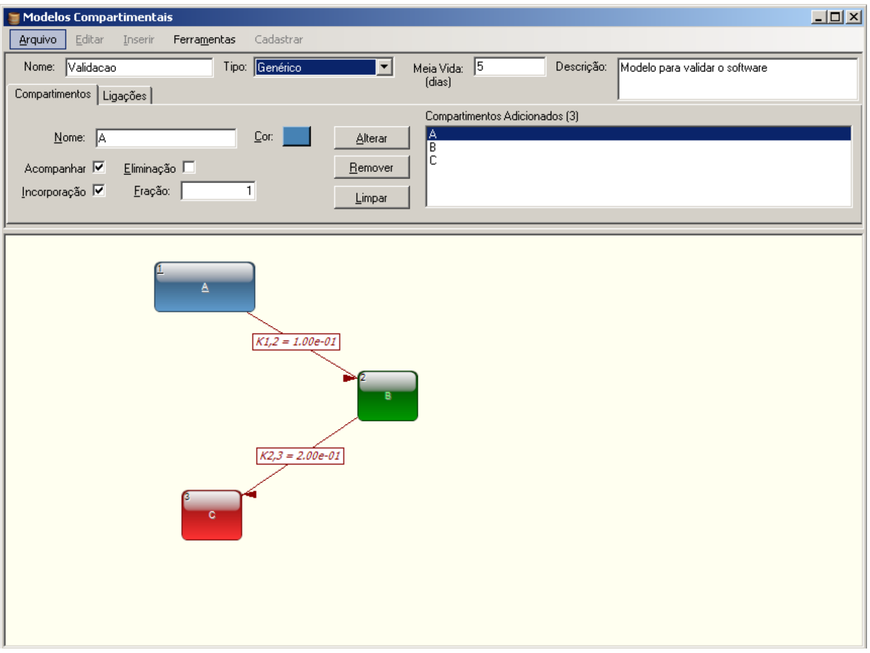
For the storage of metabolic models, it uses the Microsoft Access database, which is part of Office Professional package. Access is recommended for use in small amounts of data that would not justify the use of a large database as SQL Server or Oracle, and so was chosen as the primary data storage site.

Another way to store the models created by the program is using the XML standard, which is a format for creating documents with data organized in a hierarchical manner, totally independent of hardware or software platforms. This will allow the compartmental models be saved in this format which can be read by other applications in the future.

The HTML (HyperText Markup Language) was chosen as the standard format to carry out the values of the compartments after the resolution, thus allowing the user to save the program as an independent file. This makes possible the user to reopen it for later visualization in any internet browser without the need of CBT and SSID programs. Similarly, the graph generated with retention curves can also be saved as an image file.

2.1. Compartment Builder Tool

The CBT allows the creation and manipulation of the biokinetic models and storage it for later use. The interface of the main window, for a sample of three-compartment model is presented in Figure 2.



Nome: Validacao
Tipo: Genérico
Meia Vida: (dias) 5
Descrição: Modelo para validar o software
Nome: A
Cor: 🟦
Acompanhar ☑
Eliminação ☐
Incorporação ☑
Fração: 1
Compartimentos Adicionados (3)
A
B
C

Figure 2. CBT main screen.

The CBT screen shows two distinct areas. The bottom area shows a graphic display of the model, with the compartments represented by rectangles, their respective transfers, and the associated transfer rates. The upper area, allows the insertion and editing of data related to compartments and their links. The compartments can be moved freely in the graphic display area, with the mouse function "drag and drop", which is intuitive for any windows user.

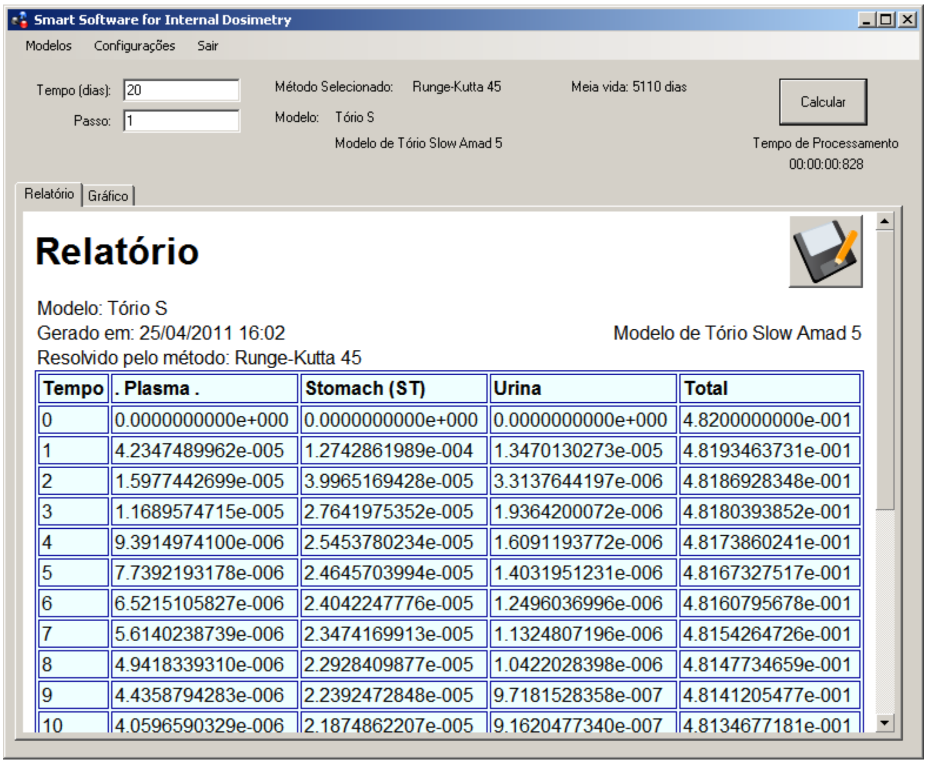
About each compartment in the model editing, you can change the following information:

- The name of the compartment
- The color, which is the line color of the graphic displayed in the resolution of the model
- If this compartment will be "monitored", ie their values will be displayed in the resolution of the mathematical model
- If it is a compartment of incorporation of the material, and therefore it is necessary to input information on the fraction of incorporating it
- If a compartment is elimination, where the values are not cumulative, as in the urine.

A second tab on this same screen allows the creation and modification of transfer´s that occur between the compartments by selecting them in two lists, containing all previously added to the model and specifying the transfer rate.

2.2. Smart Software for Internal Dosimetry

The SSID reads the compartmental models produced by the CBT and solves them using one of the mathematical methods defined, showing the values of compartments that were marked as "monitor", as shown in Figure 3, which displays a model already solved, where the columns represent the fraction of retained material in the compartment at time t, and in cases of a compartment elimination the displayed value is the accumulated activity in the time interval t-(t-1).



Tempo (dias): 20
Passo: 1
Método Selecionado: Runge-Kutta 45
Modelo: Tório S
Modelo de Tório Slow Amad 5
Meia vida: 5110 dias
Tempo de Processamento
00:00:00:828

Relatório

Modelo: Tório S
Gerado em: 25/04/2011 16:02
Resolvido pelo método: Runge-Kutta 45
Modelo de Tório Slow Amad 5

Tempo	. Plasma .	Stomach (ST)	Urina	Total
0	0.0000000000e+000	0.0000000000e+000	0.0000000000e+000	4.8200000000e-001
1	4.2347489962e-005	1.2742861989e-004	1.3470130273e-005	4.8193463731e-001
2	1.5977442699e-005	3.9965169428e-005	3.3137644197e-006	4.8186928348e-001
3	1.1689574715e-005	2.7641975352e-005	1.9364200072e-006	4.8180393852e-001
4	9.3914974100e-006	2.5453780234e-005	1.6091193772e-006	4.8173860241e-001
5	7.7392193178e-006	2.4645703994e-005	1.4031951231e-006	4.8167327517e-001
6	6.5215105827e-006	2.4042247776e-005	1.2496036996e-006	4.8160795678e-001
7	5.6140238739e-006	2.3474169913e-005	1.1324807196e-006	4.8154264726e-001
8	4.9418339310e-006	2.2928409877e-005	1.0422028398e-006	4.8147734659e-001
9	4.4358794283e-006	2.2392472848e-005	9.7181528358e-007	4.8141205477e-001
10	4.0596590329e-006	2.1874862207e-005	9.1620477340e-007	4.8134677181e-001

Figure 3. SSID main screen after the resolution of a model.

3. VALIDATION

In the current version of the program, four methods of solving systems of differential equations are presented, which makes it possible to evaluate the accuracy and processing time of each of these methods. The SSID provides a new version of the proposed implementation by Rodrigues [3] for the semi-analytical method created by Birchall [4] and three numerical methods for solving systems of differential equations presented in the library obtained in DotNumerics [5].

To validate the program, were added the metabolic models to Uranium 234, Iodine 131 and Thorium 228. These models were solved by the SSID and the obtained results were compared with the values provided by ICRP. In all cases the values were strictly identical. The choice of these radionuclides was based on the differences between their models, so while uranium has a long half-life and a slow process of absorption, iodine, in its turn, have short half-life and fast absorption.

Figures 4 shows a graph generated by SSID after the resolution of the iodine model with retention curves of plasma and thyroid for 200 days.

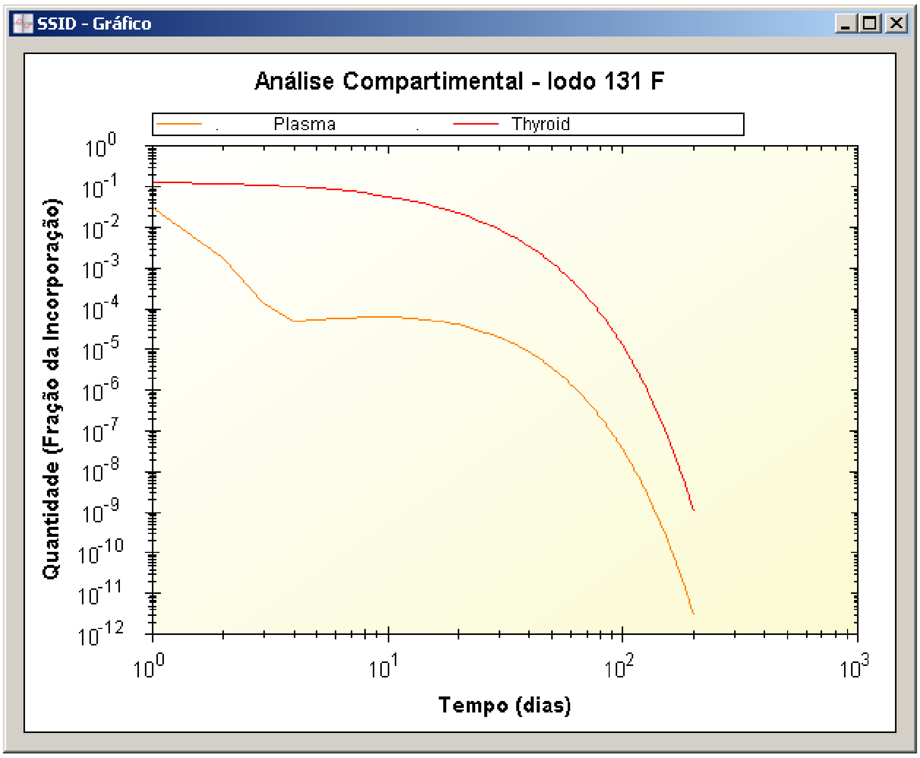


Figure 4. Graph of iodine generated by SSID.

The figure 5 presents a graph generated by SSID with the retention curves of thorium for plasma and stomach and also the curve of excretion of urine for 300 days.

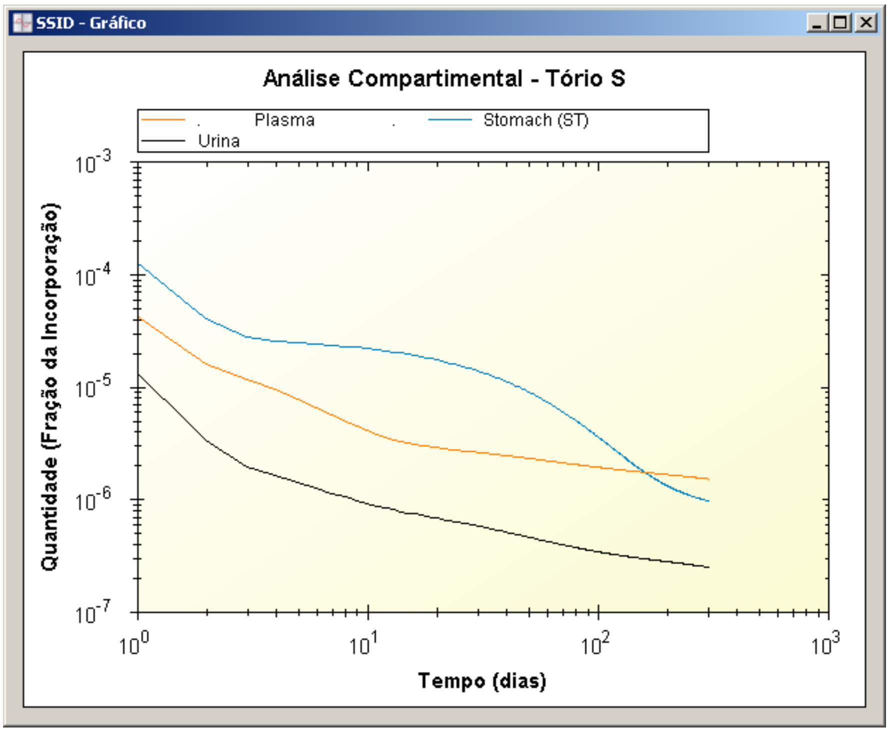


Figure 5. Graph of thorium generated by SSID.

4. CONCLUSIONS

The results obtained show the efficiency of software for solving compartmental models using systems of differential equations, thus achieving the objective of the work. During implementation of studied models, it became evident that the creation process of the compartmental model was greatly facilitated with the use of this software, as well as occasional adjustments on its structure. The use of CBT as a general tool for the construction of compartmental models, with its characteristics of data exchange with other applications by the XML standard, allows the development of other computer codes that replace the SSID with specific focus on other applications. An example is the study of pollutant dispersion in an environment, or even on the pharmacokinetics, which also makes use of compartmental models to evaluate the retention time of a drug in the body.

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