Visual Monte Carlo in-vivo – user manual

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1. Introduction

This help file describes Visual Monte Carlo in-vivo and explains the steps necessary to run VMC in-vivo calculations. VMC in-vivo was written with the objective of calculating of calibration factors in Bq/net cps for in-vivo bioassay laboratories. Voxel phantoms of the human body, of BOMAB phantoms, lung phantoms, head phantoms and knee phantoms are provided.

Radionuclides useful for in-vivo bioassay are available. Work on and validation of VMC in-vivo started in 1998 and has continued to the present day.

2. Windows compatibility

VMC in-vivo is written in VB6 (32 bits), and I am working on the up-grade to Visual studio VB14 (64 bits). Although Windows states that all programs are "backward compatible", this is not always true and it is advisable to follow the next steps to avoid any running problems. After the setup has been run, click with the right mouse button on the VMC executable, click on the page for compatibility and fill in the following:

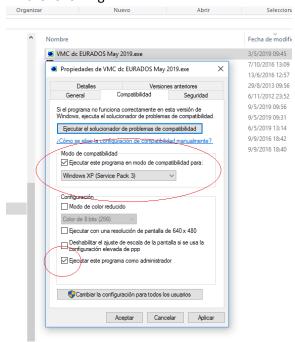


Figure 1. Compatibility setting for VMC in-vivo for Windows 7 or 10.

3. How to get started

On the first page there are three options, to create a new project, to open an existing project or to exit the program. The configurations of an existing program are saved in a dedicated text file and can be opened at any time to repeat a run.

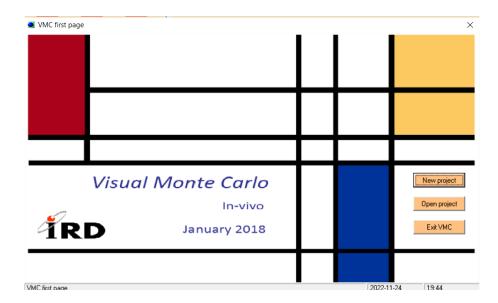


Figure 1. First page of VMC in-vivo

If the button "new project" is chosen the following screen opens, see Figure 2:

Phantom

First [1] choose the phantom that comes closest to the real object you want to simulate. Available phantoms are the ICRP male and female adult phantoms, the ANSI BOMAB, the Cincinatti University knee, the LLNL lung and two head phantoms. A saggital image of the chosen phantom will appear [2].

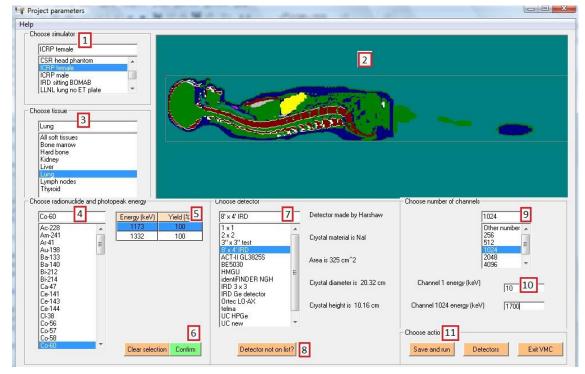


Figure 2. Define the new project

Tissues

Depending on the phantom chosen, a selection of possible tissues is presented [3]. Choose the tissue in which you want to simulate a homogeneous activity. To simulate the presence of a radionuclide in more than one tissue please send the details to my email address, johngahunt@gmail.com

Radionuclides

As soon as the tissue has been selected, a choice of radionuclides is shown [4]. In all cases, it is considered that the radionuclide is in equilibrium with its daughters. For example, in the nuclear transformation $^{137}\text{Cs} \rightarrow ^{137}\text{Ba}$ (stable) there are three possible paths and in one path the ^{137m}Ba emits a 0.662 MeV photon. The yield of this photon per nuclear transformation of ^{137}Cs is 0.846, signifying that in 100 nuclear transformations of ^{137}Cs , on average around 85 transformations will emit a 0.662 MeV photon.

Each history simulated in VMC in-vivo represents the photon emission due to one Becquerel or one nuclear transformation of the chosen radionuclide, followed by the relevant nuclear transformations of its daughters. It is therefore possible to simulate one history of ¹³⁷Cs, and no photon be emitted. In this case, by chance, the ¹³⁷Cs decayed to ¹³⁷Ba without emitting a 662 keV photon.

The three natural decay chains are included. A "short" $^{238}U \rightarrow ^{90}Th \rightarrow ^{91}Pa \rightarrow ^{234}U$ chain is also included. It is assumed that the radionuclides in a chain are in secular equilibrium. If a mixture of more than one radionuclide is required, please send the details to my email address.

Photon energies and yields

After the radionuclide has been chosen, a table will appear with the photon energies and their respective yields [5]. Photon energies with an intensity above 1% and energy above 15 keV are included. The chosen photon energy is considered by VMC in-vivo to be the photopeak energy, and VMC in-vivo will calculate the calibration factor for that energy.

For gamma spectrometry with high resolution germanium semiconductor detectors, only one energy should be chosen. The photopeak you would choose for a real measurement is the correct choice, normally the peak with the highest yield. For the ⁶⁰Co example, probably the peak with the highest counting efficiency, 1173 keV, should be chosen. It is possible to choose both energies, and in this case the net cps counted in the detector for both peaks should be used for comparison. It is however necessary to click on at least one photon energy and the chosen energy value and yield will turn to blue. To finalize, the button Confirm [6] should be pressed.

For NaI detectors, the choice can be more complicated due to the low resolution of the scintillator crystal. As an example, 133 Ba is used to substitute 131 I for calibration of in-vivo measurements. An example of the gamma spectrum of 133 Ba obtained with an 8" x 4" NaI scintillator as shown in Figure 3 below.

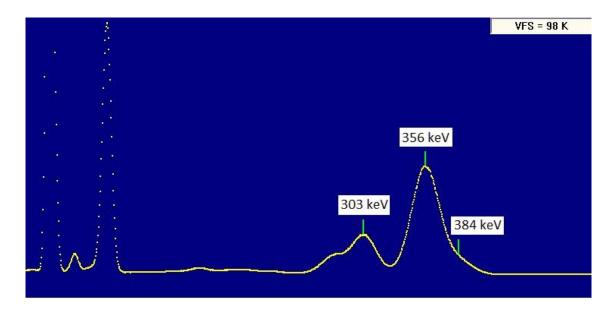


Figure 3. VMC in-vivo spectrum of a point source of Ba-133 as seen by an 8" x 4" Nal.

The peak shown at 356 keV is in fact a summation of two peaks, one with an energy of 356 keV and a yield of 62.1%, and a second with an energy of 384 keV and a yield of 8.94%.

If the Region of Interest (ROI) in the real measurement covers both peaks (approximately from 325 keV to 410 keV) then in the table of energies and yields, it is necessary to mark two photopeak energies, as shown below in Figure 4.

If the two photopeaks are selected then a photon with either 356 keV or 384 keV that deposits all its energy in the crystal will be considered as "one point in the photopeak", and the two yields are automatically summed for the calibration factor calculation.

One, two or more photopeak energies may be chosen, but there must not be a "gap" between the energies, as the ROI has to be continuous. If there is a gap, a warning message will appear.

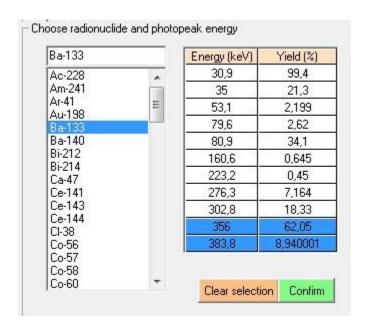


Figure 4. Selecting two Ba-133 photopeak energies for the NaI project.

To finalize, the button Confirm [6] should be pressed.

Detectors

The next step is to choose the detector [7]. VMC in-vivo comes with a folder C:\VMC in-vivo\Detectors which contains a number of text files, each with a detector description. An example of a detector file is shown in Figure 5.

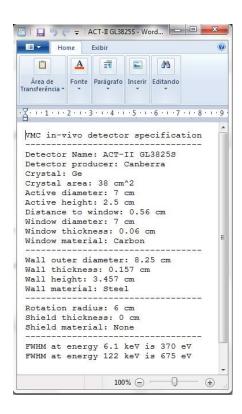


Figure 5. The detector file for detector ACT-II GL38255

If the detector you want to simulate is not on the list, it is necessary to define it [8] and give it a name. How to include a new detector is shown in Appendix A.

Multi-Channel Analyzer

VMC in-vivo simulates the spectrum obtained by the source and detector. This spectrum is not used in the calculation of the calibration factor, and is more for visual comparison of the VMC in-vivo spectrum with the real spectrum. Please remember that the VMC spectrum, which is saved to a spectrum file in the folder c:\VMC in-vivo\Spectra, does not include the background spectrum. If necessary, the background spectrum for the same counting time may be added to the VMC in-vivo spectrum using EXCEL or a similar spreadsheet.

To end the definition of the new project, the number of spectrum channels may be chosen [9]; usually a spectrum with 1024 channels shows an acceptable level of detail (see Figure 3). The energy of the first and last channels should be defined [10]. For NaI spectra, please take into account the lower resolution, so for a ¹³⁷Cs spectrum being counted, I would suggest establishing the last channel energy at around 800 keV. The MCA screen allows the establishment of ROIs and to zoom in to a part of the spectrum.

Saving the project

Once the above project information has been established, click on the button Save and Run [10]. The screen shown in Figure 6 will open. Choose an appropriate project name. The project data, including the final detector position will be saved in this project file. When you click on "Save" the project will be saved to disk

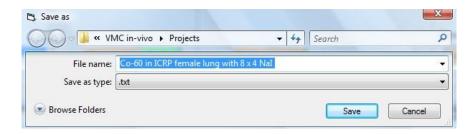


Figure 6 the save project screen.

Setting up the counting geometry

After the project has been saved, the screen shown in Figure 7 will open.

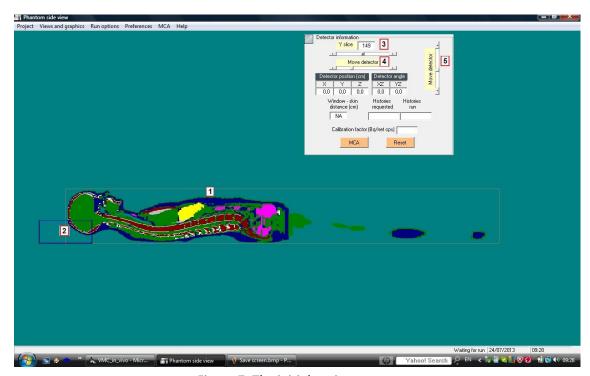


Figure 7. The initial project screen.

The ICRP female phantom is shown in saggital (side) view [1]. The 8" x 4" NaI detector is shown placed at the origin of the X, Y, Z axis system [2]. It is possible to scan through the phantom by clicking on the Y slice bar [3]. The Y slice number is shown in the box. The detector may be moved right-left by clicking on the Move Detector bar [4] or up and down by clicking on the vertical bar [5] The X, Y, and Z positions are shown on the "Detector information" frame.

The following three figures show the X, Y, Z axis system used in VMC in-vivo.

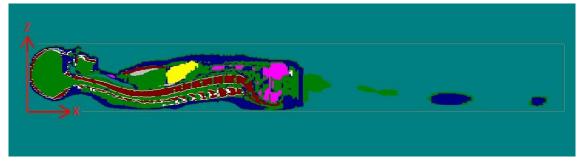


Figure 8. Saggital (side) view showing X and Z axes.

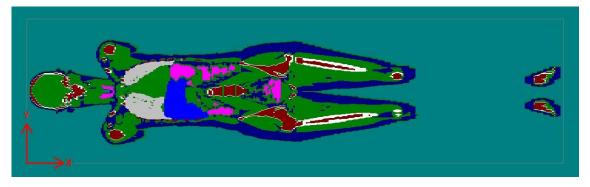


Figure 9. Coronal (top) view showing X and Y axes.

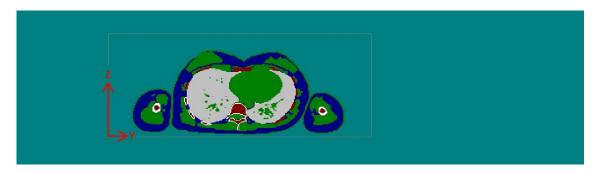


Figure 10. Transverse (front) view showing Y and Z axes.

The detector may now be positioned relative to the phantom. The same counting geometry as used in the real count should be approximated as far as possible.

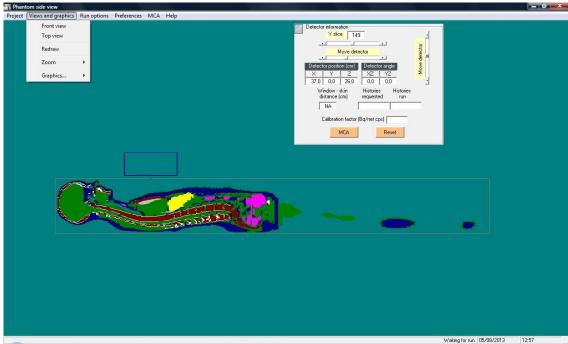


Figure 11. Positioning the detector in side view

As a suggestion, move the detector along the X axis and Z axis so that the window center is approximately in the correct position. Then click on "Views and graphics" \rightarrow "Front view to obtain the following graphics:

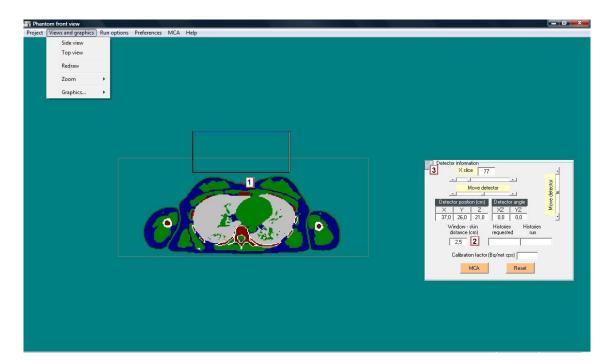


Figure 12. Positioning the detector in front view

The moving red point [1] on the phantom represents the point that the center of the detector window is pointing at; consider that there is a laser beam pointing along the center line of the detector. VMC in-vivo calculates the distance between the center point of the window detector and the skin or surface of the phantom. This distance is shown on the "Detector information" frame [2]. It is possible to drag and drop the "Detector information" frame so as to position it away from the phantom and detector [3].

Clicking on "Views and graphics" \rightarrow "Top view will obtain the graphics shown in Figure 13.

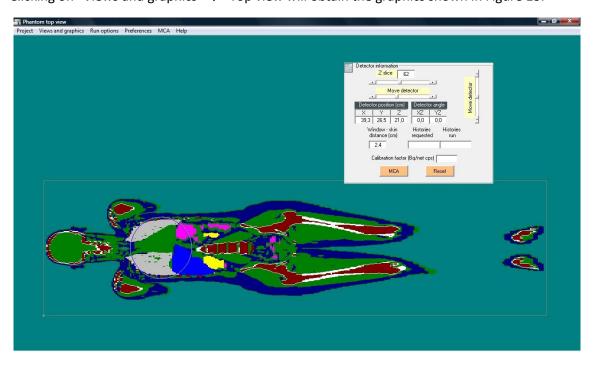


Figure 13. Positioning the detector in top view

Alternating between the top, front and side views will enable the VMC in-vivo detector to be positioned within a millimeter or two to the correct or "real" position.

4. Making the run

The project has been defined - it's time to calculate the calibration factor. To start the run, choose the number of histories required from the menu "Run options" \rightarrow "Run 10,000 histories". 10,000 histories may be used for a quick check or demonstration, 1,000,000 histories may be used for a rough estimate of the calibration factor. 10,000,000 histories may be used for a full calculation run. Each history represents one Bequerel; one nuclear transformation of the radionuclide is simulated. The more histories run, the more precise is the calculation of the calibration factor. However, usually after 5,000,000 histories the calibration factor will not change by more than 1%.

When the program is running, the graphics shows where the photon started, it's initial direction, and any photoelectric (yellow circles) or Compton (blue circles) interactions in the phantom or in the detector. Interactions in the detector window are shown in white. In the menu "Views and graphics" \rightarrow "Graphics" \rightarrow "Show start point only" it is possible to show only the photon start point in the phantom.

The graphics option slows down the run considerably, therefore for longer runs (R > 100,000) it is recommended to turn the graphics off. A run of 10,000,000 histories on a "fast" laptop computer with the graphics turned off takes around 2 $\frac{1}{2}$ hours. The number of histories run is shown on the "Detector information" frame. The run ends when the number of histories requested is equal to the number of histories run.

The results

The main objective of all this work is to determine the calibration factor for the geometry and radionuclide in question. The calibration factor in Bq or kBq per net cps is shown on the "Detector information" frame. From previous results from intercomparisons, the calibration factor is calculated to within a 10% uncertainty.

Program description

VMC in-vivo is a computer program that simulates the measurement of a real person or phantom containing a radionuclide with a real detector. It uses the Monte Carlo technique to:

- Simulate the emission of photons in a "contaminated" tissue or organ;
- Transport the photons through the phantom;
- See if a photon leaving the phantom is going in the direction of the detector;
- Simulate the photon detection by the detector;
- Bin the number of photons detected in the photopeak, and
- Calculate the calibration factor

The mathematical phantoms

The human whole-body phantoms

VMC in-vivo contains the ICRP male and female reference phantoms, for a detailed description of the phantoms, see ICRP, 2009. Adult Reference Computational Phantoms. ICRP Publication 110. Ann. ICRP 39 (2). I would like to acknowledge here the kind permission granted by the ICRP to distribute the two phantoms in this program. For VMC in-vivo, the ICRP voxel phantoms were modified by the "blending" of organs and tissues considered to be of no interest for in-vivo bioassays. The organs defined in the phantoms are: thyroid, lung, liver, kidney, lymph nodes, adipose tissue, cortical bone, bone marrow, and "the rest" which blends together all the other organs and tissues (muscle, brain, skin, adrenals, etc.) For further protection, the ICRP phantom files have been encrypted.

For the male phantom, a whole-body clinical computed tomography image set of a 38-year-old individual with height 176 cm and mass slightly below 70 kg (Reference Male: 176 cm and 73 kg) was selected for the construction of the male reference computational phantom. The person was lying supine with the arms parallel alongside the body. The data set consisted of 220 slices of 256 x 256 pixels. The voxel size is 8 mm in height with an in-plane resolution of 2.137 mm for the male.

The female reference computational phantom was based on the computed tomography scan of a 43-year-old individual with height 167 cm and mass 59 kg (Reference Female: 163 cm and 60 kg). The final data set consisted of 346 slices. The voxel size is 4.84 mm in height with an in-slice resolution of 1.775 mm.

The Yale phantom

As an option for the male phantom, VMC in-vivo contains a male voxel phantom produced at Yale University, see http://noodle.med.yale.edu/zubal/. A voxel phantom with a format of 488 "slices" each of 192 x 96 picture elements is used. The size of each voxel is 3.6 mm x 3.6 mm. The voxel phantom is derived from a whole body magnetic resonance image (MRI) scan and was obtained from the Yale University voxel phantom library that is maintained by George Zubal, PhD. The voxel phantoms in this library are freeware.

The Yale voxel phantom was modified at the IRD so as to maintain only the tissues relevant for WBC laboratories: cortical bone, bone marrow, lungs, thyroid, liver, kidney and the rest, comprising all other organs and tissues.

The BOMAB

The BOMAB phantom is based on the ANSI-N13.35 standard specifications and is made up of 3 mm x 3 mm x 3 mm voxels. There is only one tissue - BOMAB tissue, of density equal to 1.0 g/cm³. In the current program, the BOMAB is in the horizontal position but the voxel BOMAB may also be configured into a sitting position. A 95% percentile BOMAB is also available.

The BOMAB phantom in VMC in-vivo was validated in the IAEA activity intercomparison of 2005.

The knee

A knee voxel phantom representing a human left knee has also been included in VMC in-vivo. The knee is based on a computerized axial tomography of the Spitz anthropometric knee phantom. The tissues included are bones and muscle tissue. The voxel size is 2 mm x 2 mm x 2.5 mm. The phantom has 150 slices. VMC in-vivo and the knee phantom were validated in the international EURADOS intercomparison J. M. Gomez-Ros, J. G. Hunt et al. *Monte Carlo modelling of Germanium detectors for the measurement of low energy photons in internal dosimetry: Results of an international comparison*. Radiation Measurements (43, 2-6), pp. 510-515 (2008). VMC in-vivo was participant "n".

https://www.sciencedirect.com/science/article/abs/pii/S1350448707005811

The Lawrence Livermore National Laboratory lung phantoms

The Lawrence Livermore National Laboratory (LLNL) lung phantom is also included, with and without the overlay. The LLNL phantoms are based on a computerized axial tomography image of the real LLNL lung phantom. For both phantoms, the voxel resolution is 2 mm x 2 mm x 2 mm. there are 256 slices in the voxel phantom. The tissues defined are lung, hard bone, axillar lymph nodes and the rest, consisting of skin, muscle, fat, etc. VMC in-vivo and the lung phantom were validated in the international EURADOS intercomparison D. Broggio, J. G. Hunt et al. *Monte Carlo modelling for the in vivo lung monitoring of enriched uranium: Results of an international comparison*. Radiation Measurements Vol 47(7) pp. 492-500. (2012). VMC in-vivo was participant "I".

https://www.sciencedirect.com/science/article/abs/pii/S1350448712001400

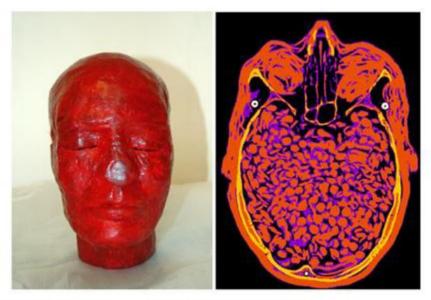
The BPAM head phantom

The BPAM head phantom is based on USTUR scan of BPAM-001 and there are 184 slices of height 1.25 mm with in-slice resolution of 203 x 226 at 0.949 mm \times 0.949 mm. VMC in-vivo and the BPAM and Bfs head phantoms were validated through an international EURADOS intercomparison "EURADOS intercomparison exercise on MC modelling for the in-vivo monitoring of AM-241 in skull phantoms Part I, Part II and III)" see links below. VMC in-vivo was participant P17.

https://www.sciencedirect.com/science/article/abs/pii/S0969806X13006579 https://www.sciencedirect.com/science/article/abs/pii/S0969806X15001474.

The Bfs head phantom

Voxel head phantom based on artificially made phantom owned by Bundesamt für Strahlenschutz (Germany). Included in the above EURADOS head intercomparison. VMC in-vivo was participant P17.



Size of the volume $173 \times 234 \times 137$ voxels (X, Y, Z) Voxel resolution $0.78125 \times 0.78125 \times 1.5$ mm

Orientation

Z axis is from the top (slice 0) to bottom of the head (136)
X axis is from the left to the right (left side on the picture is left side in real)
Y axis is from top (anterior part of the skull) to the bottom (posterior part of the skull)

The radionuclides

The most common radionuclides of interest to in-vivo laboratories are included in the list box of radionuclides. Each radionuclide is characterized by all photon (X ray and gamma) emissions above 20 keV and with a yield above 1%. Exceptions to these restrictions are made for some important radionuclides such as Pu-238 and Pu-239. Exact photon energies, for example of 1.5 MeV with a yield of one may also be entered by choosing En-1.5 MeV.

The Monte Carlo program and RANMAR

VMC in-vivo is designed specifically for voxel geometries and has an extensive graphic output. It is written in Visual Basic version 6. As the energies of the radionuclides of interest for WBC laboratories fall in the range of 0.01 - 1.5 MeV, only photoelectric and Compton interactions are considered. The Monte Carlo code uses the RANMAR random number generator, with a period of approximately 10³⁰ random numbers – more than sufficient.

APPENDIX A - Define a new detector

The VMC in-vivo SETUP comes with a selection of previously defined NaI and Ge detectors as text files in the folder C:\VMC in-vivo\Detectors. It is necessary to include the detectors you use in your laboratory to simulate your counting geometry and detector. To include a new detector, it is necessary to start a new project, define the phantom, radionuclide and photopeak energy. When it comes to choose a detector, push the button "Detector not on list?"

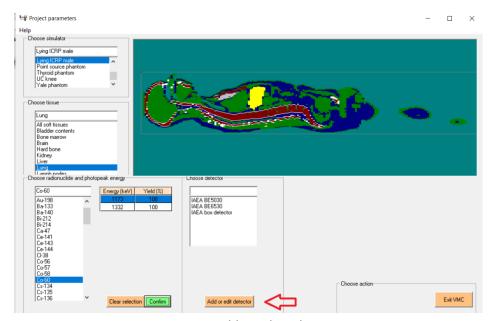


Figure A1. Add or edit a detector

The following screen will appear:

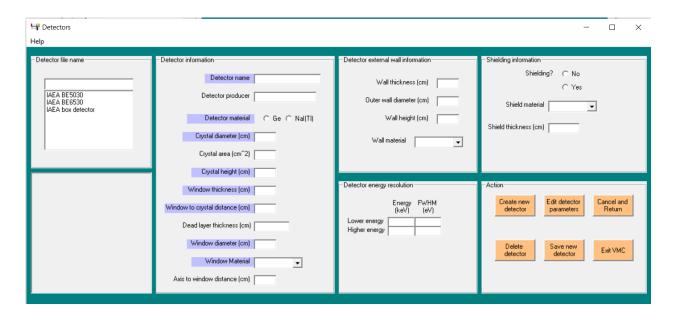


Figure A2. Define the new detector

I will use the example of the Canberra Model 802 Scintillator detector as an example of how to fill in the screen. The eight most important fields to fill in are indicated in purple. The detector

name identifies the detector for VMC in-vivo. The crystal material, diameter and height, window material etc. are given in the detector specifications or should be requested from the supplier. The MIRION BE3830 is used as a worked example from the site:

https://mirionprodstorage.blob.core.windows.net/prod-20220822/cms4 mirion/files/pdf/spec-sheets/ops-1424 bege spec sheet.pdf?1579456901



SPECIFICATIONS

BEGe DETECTOR

General Specifications and Information

Standard configuration includes:

- Vertical Slimline" dipstick cryostat with 0.6 mm Carbon Composite window and 30 liter Dewar.
- Model iPA Intelligent Preamplifier with 3 meter bias, high voltage inhibit, signal and power cables.

Other cryostat options consult web site.

Relative efficiency is a *typical value*, not a spec limit.

Model Number	Area (cm²)	Thickness (mm)	Typical Rel. Eff. (%) ≥	Full Width Half Max (FWHM) Resolution (keV)			Endcap
				At 5.9 keV energy	At 122 keV energy	At 1332 keV energy	diameter mm (in.)
BE2020	20	20	9	0.35	0.65	1.80	76 (3.0)
BE2820	28	20	13	0.40	0.70	1.90	82 (3.25)
BE2825	28	25	18	0.40	0.70	1.90	82 (3.25)
BE2825P	28	25	18	0.35	0.65	1.80	82 (3.25)
BE3820	38	20	20	0.45	0.75	1.90	89 (3.50)
BE3825	38	25	26	0.45	0.72	1.90	89 (3.50)
BE3825P	38	25	26	0.40	0.65	1.80	89 (3.50)
BE3830	38	30	34	0.45	0.72	1.90	89 (3.50)
BE3830P	38	30	34	0.40	0.65	1.80	89 (3.50)
BE5025	50	25	37	0.50	0.75	2.00	102 (4.0)
BE5030	50	30	48	0.475	0.72	2.00	102 (4.0)
BE5030P	50	30	48	0.425	0.675	1.80	102 (4.0)
BE6530	65	30	60	0.50	0.75	2.00	114 (4.5)

If information is missing, such as the thickness of the dead-layer, a default value can be used. If the outer wall thickness is not given, ask the supplier.

For NaI detectors, reference energy resolution values are given in the following paper:

https://www.sciencedirect.com/science/article/pii/S1738573321002680

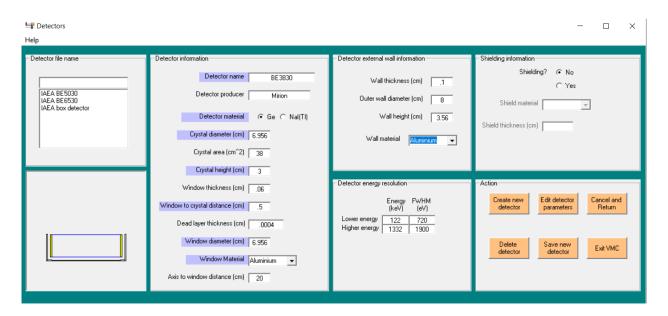


Figure A3. Fill in the detector information.

After pushing the "Save new detector" button, a txt file in the folder C:\VMC in-vivo\Detectors is created with the following format and information, see Figure A4.

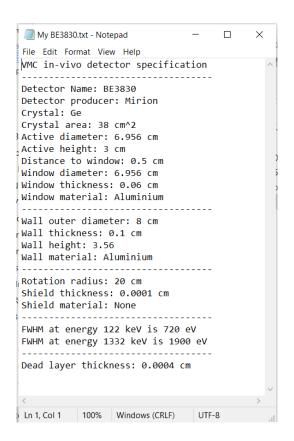


Figure A4. Txt file with name "My BE3830" with the detector information.