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# Report on the Geant4 simulations performed for the "Realisation of the Bq" project

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## 1. Introduction

The main objective of the "Realisation of the Bq at basic level" project is to develop a "fully" reproducible  $4\pi$  ionisation chamber. For this purpose, all the dimensional and operational parameters of the chamber have to be described in the construction specifications to ensure that any chamber build accordingly will display an almost identical response function. The acceptable variation of the response between two such "identical" ionisation chambers should be below 0.2% for a broad energy range (20 keV- 2 MeV).

Monte Carlo simulations have become an integral part of developing new radiation detectors and the work on the ionisation chamber that is being built as part of this project makes no exception. Until now, Monte Carlo simulations were performed at IRMM using EGS4 [1] and MCNP5 [2] and at LNHB using Penelope [3]. Some of these simulations were used to define the parameters of a prototype ionisation chamber, while others dealt with other aspects of the operation of the chamber such as the effect of the ampoules holding the source, or the positioning of the ampoule. In 2010 the work started on designing a new prototype. At the same time, a new simulation program for the project was started, using the Geant4 [4] framework.

This technical document will present the details of the simulations as they were performed using the Geant4 [4] framework, focusing on the last version of the simulation code. This document, together with the source code and the documentation included in the source code should provide enough information for anyone to reproduce the results and expand the simulations.

### **Why Geant4?**

Of the existing Monte-Carlo simulation packages, Geant4 is probably the most powerful, and at the same time the most complex. The way the package is built allows much better access to all the stages of the simulation, but at the cost of a slight increase in complexity; a bonus point is that the ROOT framework can be used to analyse the results of the simulations.

Another reason is that the geometry description is more free and closer to a natural description of the object, allowing arbitrary positioning of the geometry components (for example in scenarios where the influence of the tilting of a structural element is studied). Materials of any composition and complexity can be used, and additional properties of the detector, for example charge collection effects, can be included.

### **Purpose of the simulation program**

The main goal of the simulation program is to assist in the decision making process for the new prototype of the ionisation chamber that is currently in the design phase. Because of the reproducibility emphasis of the project the simulation program must be appropriate not only to assess the performance of the Ionisation Chamber but also to study how the performance is influenced by small deviations from the nominal values of the components.

## 2. The simulation program

The philosophy of the Geant4 framework requires the user to implement four areas of the simulation (or, in C++ terms, to provide implementations for four virtual classes): the physical processes (which allows the study of how important different interaction mechanisms are), the particle source, the geometry of the detector (the ionisation chamber) and the analysis that should be performed on the results of the simulation. Once this information is provided, the Geant4 framework will generate particles according to the implementation of the source provided by the user, will transport and make the particles interact with the detector according to the physics list and geometry and will, on an event by event basis, analyse the results.

In a typical program following the Geant4 patterns, all of these would be hardcoded in the source code. For example, all of the details of the geometry would be described in C++ language (using the classes provided by Geant4) and any modification to the geometry would require editing and recompiling of the source code. We have found that this approach is lacking for the scope of our project because of the type of studies that we were interested to perform. For example, studying the sensitivity of the response to the thickness of the inner tube of the ionisation chamber, where the result for five thicknesses are compared would require, on one hand, recompiling the code, but also modifying the description of the detector in the source code five times, at all the places where the geometry is affected. It is clear that this leads to problems in detecting any error that might occur in the process, and also makes repeating a simulation somewhat difficult. Saving the compiled executable file is only a partial solution, as the changes between compiled executables cannot be identified. To overcome this issue the implementation of the required classes was performed in a generic way, with all the numerical parameters read from external files.

During the course of the project it became obvious that the study of the way the collection of charges takes place in the IC is of the highest importance. This is traditionally left out of the Monte-Carlo simulations (whose sole purpose is to determine how and where the energy is deposited inside the detector). As a result, the analysis part of the simulation was extended to include the charge collection.

### Technical details

The programming language used by the simulation (and Geant4) is C++. The analysis takes advantage of the excellent data analysis abilities of the ROOT framework [5] (C++). Extra care was taken so that the computer code itself is as well documented as possible (doxygen [6]) The management of the versions of the code was performed using CVS [7].

The hierarchy of the external files is:

- ICsetup.inp: the master configuration file, contains the name of the files where all the other information will be read. This is the only filename coded in the program, so a file with this name must exist in the run directory (see Appendix 1 for an example of input file with description of the fields)
- files describing the simulation scenario being investigated

- file with the description of the particle source
- geometry description file
- analysis file
- file with the charge collection map
- files with description of real sources

## 2.1 The physical processes

The default physics processes used by Geant4 have been proven inadequate at the low energies of interest for the project (Geant4 was developed at CERN to be used in high-energy physics experiments). The simulation community became aware of this issue soon after the launch of Geant4 and a few groups undertook the initiative to develop interaction packages that can be used at low energy. One of these approaches rewrote the physical processes implementation from Penelope [8] and made it available in Geant4.

Our choice of low energy package is the Penelope implementation, and at all times during the simulations all the processes were kept active.

The cut-offs are also declared during this part of the simulation. In Geant4 the range cut-off represents the accuracy of the stopping position. It does not mean that the track is killed at that energy. The value of the cut-off is defined in the "ICsetup.inp" file, and, in most cases, a value of 10  $\mu\text{m}$  was used.

## 2.2 The geometry

The geometry of the detector constitutes one of the most important parts of the simulation code. Geant4 provides the user with a whole array of building blocks that can be used to generate geometries of any complexity. In principle these building blocks are used as part of the C++ code, and the geometries are "hardcoded" in the simulation.

Compared to the detectors at CERN that were the aim of the Geant4 simulation package, the ionisation chamber is a relatively simple detector. Another factor that was taken into account is that for the current project we are not interested so much on the response of the detector as we are on its sensibility to variations of the dimensions of the components of the ionisation chamber. That is to say that the goal of the simulation is not to assess the response of the chamber but to estimate the tolerances on the components.

As a result, we have decided to not hardcode the geometry in the C++ code but to implement another layer of geometry description that allows changes of the geometry without recompiling the code. This approach has also the advantage that once the source code is compiled, simulations can be run without knowledge of the inner workings of the program, simply by changing the parameters in the input file.

The geometry is described in terms of a restricted set of building blocks, which are better suited to describe the geometry of the ionisation chamber than the (more general) Geant4 building blocks. This simplification arises from the cylindrical geometry of most of the components of the ionisation chamber.

The ionisation chamber is described (following the Geant4 pattern) as a hierarchical structure of objects, where any component must be part of another one. Each of the components of the ionisation chamber is described by a single line in the input file.

An example of geometry input file and more details about how the geometry is described are presented in Appendix 4.

As a side note, the Geant4 framework allows arbitrary complexity geometries to be imported directly from CAD programs. We have found that the geometry of the ionisation chamber is too simple to justify the overhead of using this feature.

## 2.3 The particle source

The response of the IC to single energy particles forms the basis of the studies that are performed using the Monte-Carlo method. This is useful in most circumstances but it does not translate easily in methods to test whether a component of the ionisation chamber is out of specifications. To address this issue, the particle source for the simulation was written so it allows not only single energy particles, but also continuous distributions (for  $\beta^+$  and  $\beta^-$  decays) and full radionuclides, with all possible combinations of emitted particles and emission probabilities.

Each of the radionuclides are described in text files that are distributed at the same time with the source code. The list of radionuclides can be extended by supplying the appropriate isotope description file.

An example of a source input file can be found in Appendix 2.

## 2.4 The analysis

The analysis is that part of the program where the energies deposited at each interaction in a sensitive component are put together to calculate the response of the ionisation chamber. In our simulation we have implemented two types of analysis. The first one deals with the energy deposited in each of the components. The second one uses a model of the field distribution inside the chamber to analyse only the interactions in the sensitive area of the gas, and which are collected by the electrodes.

In both cases the mean deposited (or collected) energy is calculated following the analysis described in the MCNP manual [2] (and described in Appendix 5) .

### Charge collection

When dealing with detectors, the problem of charge collection is usually left aside because in most cases all the energy deposited in the detector is collected and measured. This is not the case in an ionisation chamber, where guard rings divide the sensitive gas volume defining parts that will not yield any signal in the collecting electrodes, no matter the amount of energy deposited. This effect is expected to be important because the plans for the next prototype foresee a number of such dead volumes.

In the case of an ionisation chamber we can safely assume that any charge generated in the collection area of the gas will be collected. This is not entirely true, but the high intensity of the field due to the high voltage will decrease the influence of the charge losses through recombination .Also, as we are interested in the variation of the response between two identical chambers, we are assuming that the variation in losses between such two chambers is negligible for the scope of the project.

The charge collection was included in the simulation as an additional step of the analysis of the interaction in the materials. For each interaction that takes place in the gas we are interested to find out where the charges are collected: the electrodes, the

guard rings or the other structural elements. For that, a finite-element method (FEM) software (ELMER [9]) was used to calculate the field distribution in the chamber. Taking advantage of the cylindrical symmetry of the ionisation chamber, the FEM method is used in a two-dimensional space, made by half of the cross-section through the IC, and the tracking of particles in this field is performed in Geant4.

Unless otherwise specified, in the following section, the response of the chamber refers to the energy deposited in the "collectable" region of the gas, and not to the energy deposited in the total gas volume.

More details about the charge collection procedure can be found in Appendix 6.

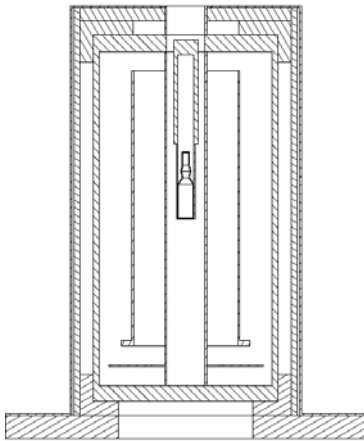


### 3. Simulation results

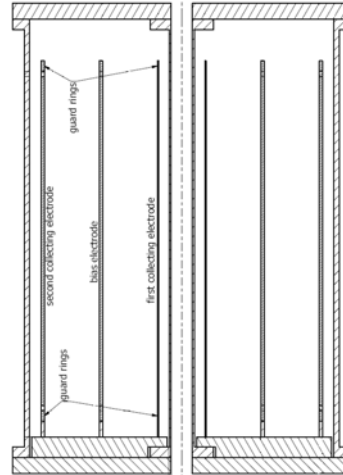
In this chapter some of the results of the simulations will be presented. The goal of the simulations is to study the design of the new prototype, but in some cases the existing prototype (the RWD chamber) was used.

Without going in the details of the differences between the two designs, the following pictures present the schematic drawings of the two chambers, as they were used in the simulations.

**Figure 1: The RWD design**



**Figure 2: The IC2010 design**



#### 3.1 Comparison with previous simulations

In this section we will present two comparisons between results obtained with the simulation code developed using Geant4 and results obtained previously in the project in order to verify the correctness of the code implementation.

##### 3.1.1 Response to mono-energetic photons

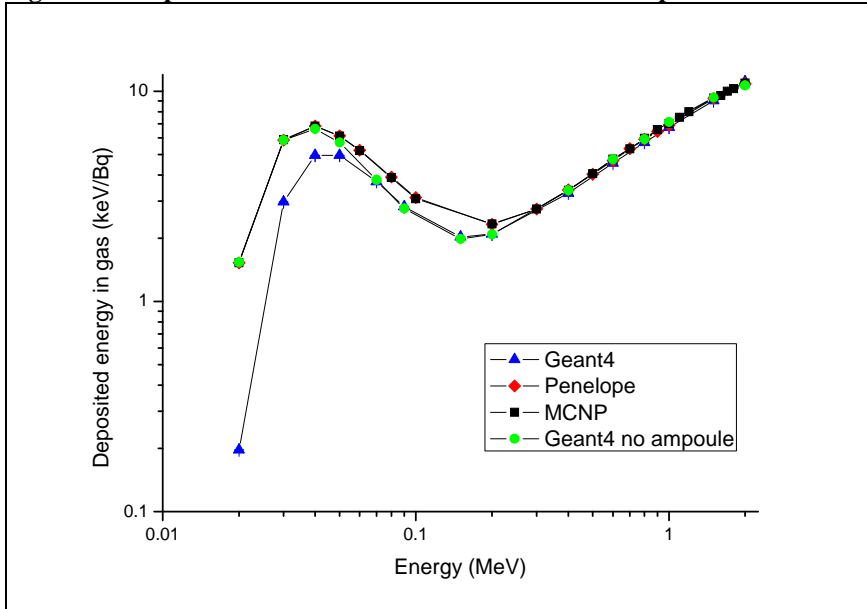
Previously [10], the results of Monte-Carlo simulations using MCNP5 and Penelope were compared for the case of a simple geometry and a good agreement was found between them. While a full comparison between our code in identical conditions might seem justified, it would only replicate some of the in-depth studies comparing the available Monte-Carlo codes [11]. As a result we have opted for comparing the results of the real geometry of the prototype obtained with Geant4 with those of a similar (more simple) geometry used in the previous comparison (where only the vertical components of the prototype were included).

In addition to the geometry difference, for the Geant4 simulation we have used two type of sources:

- point-like mono-energetic gamma source (similar to that used in the previous comparison)
- a more realistic mono-energetic source: the described source consists of mono-energetic emitters dissolved in water, contained in an glass ampoule (uniform distribution of source emitters from a "water" cylinder, surrounded by the ampoule)

The results of the comparison can be seen in figure 3. It can be seen that the results are in agreement at low energy where the energy deposition is limited to the volume in the center of the chamber (far away from the regions of difference between the geometries) and at high energies, where the deposited energy depends the least on the geometrical details of the chamber and more on the total mass of gas present in the chamber.

**Figure 3: comparison between Geant4 and MCNP/Penelope simulations**



Another aspect that becomes clear from these simulations is the huge effect that the ampoule and the water solution that contains the source have on the response of the chamber.

### 3.1.2 Tolerance on the thickness of the inner wall if Al is used

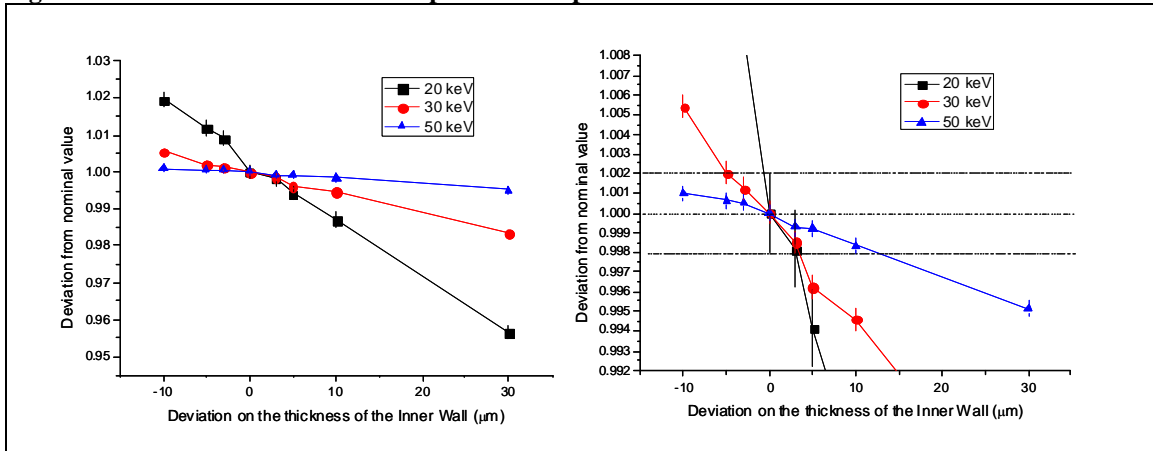
The tolerances on machining the inner wall of the ionisation chamber are among the critical parameters in achieving the required 0.2% reproducibility because of the high attenuation rate at low gamma energy. This is why these tolerances were previously studied to a great extent [10], using both an analytical model and MCNP5. For both this reasons, performing the same study using the Geant4 code is one of the most important tests that a successful simulation program needs to pass.

Simulations were performed for the prototype chamber using a point-like mono-energetic gamma source. The only parameter that was modified between the simulation runs was the thickness of the inner wall. Seven simulation runs were performed, starting with the nominal thickness of 2mm and using both higher and lower thicknesses with a deviation of a few  $\mu\text{m}$  from the nominal value ( $\pm 3 \mu\text{m}$ ,  $\pm 5 \mu\text{m}$ ,  $\pm 10 \mu\text{m}$  and  $30 \mu\text{m}$ ). The study used only low energy photons ( 20 keV, 30 keV and 50 keV) because the effect on the response is decreasing with increasing energy.

Figures 4 show the results of the simulation. The figure on the left side shows the full results, while the one on the right shows a detail concentrating on the results around the nominal value. In the second figure we represented with dashed line the 0.2% accepted deviation on the response that is deemed acceptable for the project. It can be seen that the curve corresponding to 20 keV intersects this curve very close to the nominal values, in agreement with the  $2 \mu\text{m}$  tolerance at 20 keV obtained in the previous

studies. It can also be seen that the tolerance increases rapidly with increasing energy, so that a tolerance of roughly  $12\mu\text{m}$  is needed to fulfil the goal of the project at 50 keV.

**Figure 4: deviation from the ideal response in the presence of deviations of inner wall thickness**



### 3.2 Studies concerning the thickness of the inner wall of the ionisation chamber

The thickness of the inner wall of the ionisation chamber was identified as one of the bottle necks in successfully fulfilling the goals of the project. This is due to the fact that achieving  $2\mu\text{m}$  tolerance on what is basically a tube 40 cm long, inner diameter of 3 cm and a wall thickness of 2 mm is beyond any existing machining possibility.

To address this issue we have investigated a number of possibilities, using both simulations and enquiring about manufacturing procedures. This section focuses on the results of the simulations for these scenarios.

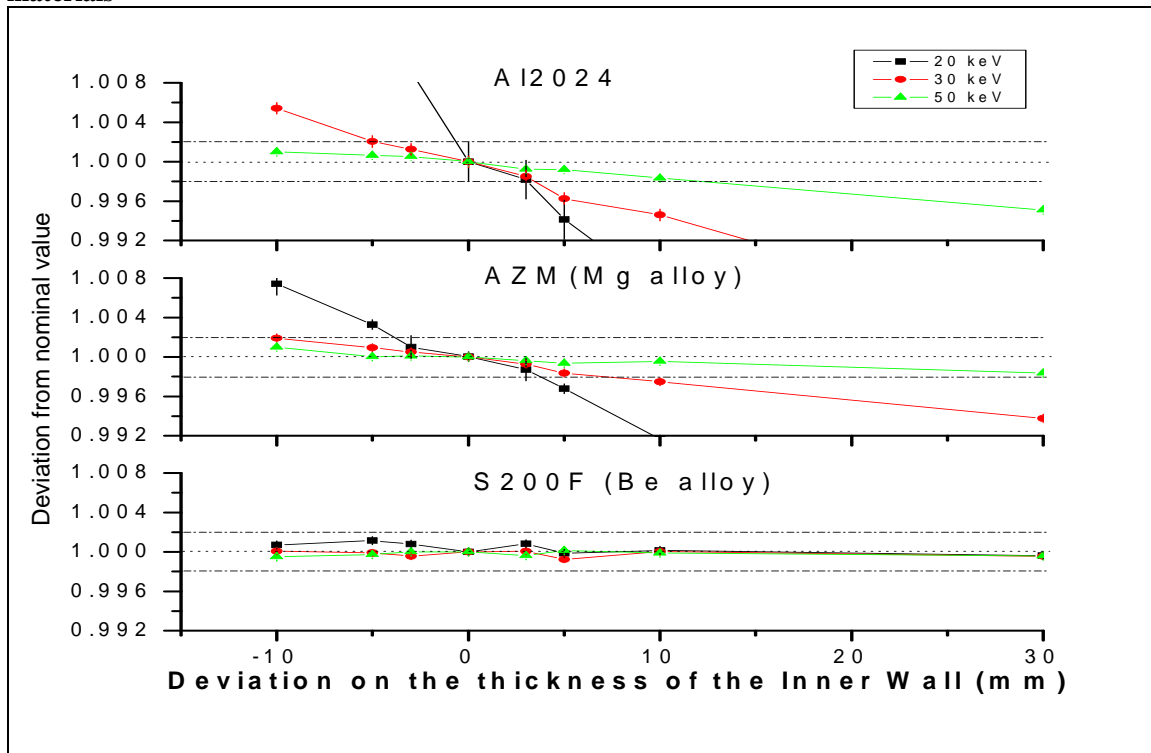
#### 3.2.1 Tolerance on the thickness of the inner wall if other materials can be used

The first scenario that was investigated is the possibility to have the inner wall of the ionisation chamber made of a different material instead of Aluminium. It is obvious that the only way to ease the tolerances on the thickness is to use a material with lower absorption than Aluminium, which can only be achieved by using a material (or alloy) with a lower atomic number. Another critical constraint is that the ionisation chamber needs to be pressurised to 2 MPa, so the material should be mechanically strong. After a search of the materials available on the market we found two other materials that seem fit for the purpose: AZM [12], a Mg-Al alloy used in aeronautics and a Be-Al alloy (S200F [13]) that can be used for structural components.

Simulations to establish the required machining tolerances were performed for all three possibilities: Aluminium, AZM and S200F.

The figures below show the variation of the response, as a function of the deviation from the nominal values of the thickness of the inner wall for the three materials. The horizontal dotted lines denote the acceptable limits for the project (0.2%).

**Figure 5: influence of the deviations from design values of the the inner wall thickness for different materials**



It can be seen that compared to Al, the use of AZM is a much better solution (5  $\mu\text{m}$  tolerance), while the use of Be would remove any constraint on the tolerance of the inner tube, Practically, if Be is used, the response is independent of the thickness of the tube for the interval we have studied. (Employing the analytical model, the required tolerance for a Be inner wall is of the order or 100  $\mu\text{m}$ ).

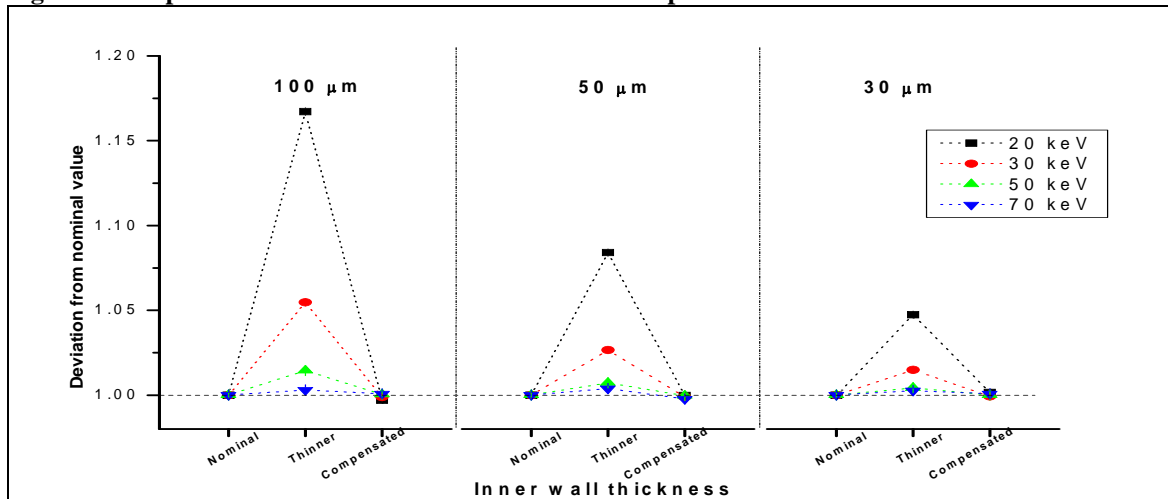
While this approach seems to solve the problem of the tolerance of the inner wall there are still a number of concerns of which we will only mention two: the very high price of the Be-Al tube and the toxicity of Be.

### 3.2.2 The use of compensation Al foils

Another work-around envisaged for the problem of having technically unachievable tolerances for the inner tube thickness is to employ thin aluminium foils, which would surround the ampoule or the holder to compensate for the thickness differences between chambers. The purpose of the simulation was to see whether such an approach would give the required results.

Three scenarios were studied, each for four energies (20 keV, 30 keV, 50 keV and 70 keV) . In each of the scenarios, the response of the chamber for a thinner inner wall was compared with the nominal response and with the the response obtained by adding a thin Al foil to compensate the difference. The three scenarios assumed a difference between the real thickness and the nominal thickness of 30  $\mu\text{m}$ , 50  $\mu\text{m}$  and 100  $\mu\text{m}$ . The three deviation values that were used in this case correspond to estimated realistic tolerances for the inner wall of the prototype.

**Figure 6: compensation of the inner wall deviations if compensation foils are used**



As it can be seen from the figure above, compensating the thickness of the inner wall with thin Aluminium foils is a viable procedure, and that a properly measured foil can compensate for the deviations in machining the inner wall. Of course, this approach has a few drawbacks in itself: while much higher machining precision can be achieved in machining the compensation foil, it is almost impossible at this time to measure how thick it should be, because measuring the thickness of the inner tube is a very complicated issue. Also, this approach will add to the complexity of the operation of the ionisation chamber because another component (the compensation foil) needs to be taken care of while manipulating the source. More issues can be foreseen when the replacement of the foil has to be performed.

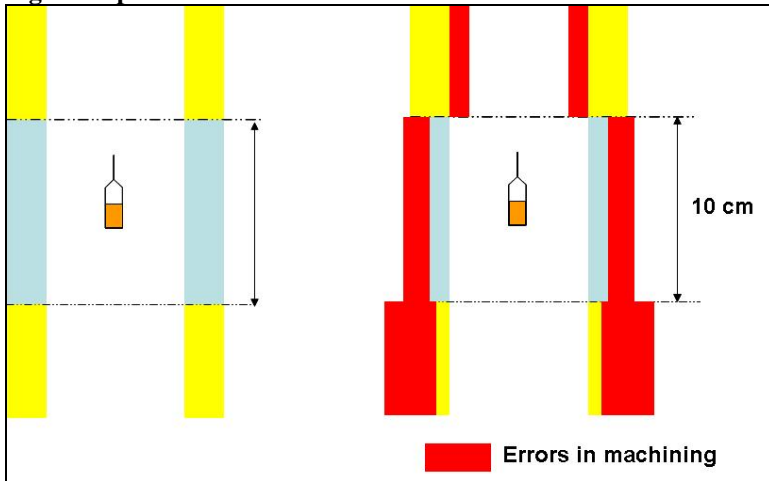
### 3.2.3 Inner tube made of three sections machined to different tolerances/accuracies

The purpose of the simulation presented in this section is to investigate whether the inner tube can be made of three shorter sections, each of them easier to machine, which are then welded together.

This idea has its basis in the fact that the two dimensional maps show that most of the response comes from photons that went through the inner tube in a rather narrow region around the position of the ampoule. Another starting point for the simulation was given by the fact that the much better tolerances can be achieved on machining a 10 cm long tube, which is then welded to other pieces to form the inner tube of the ionisation chamber.

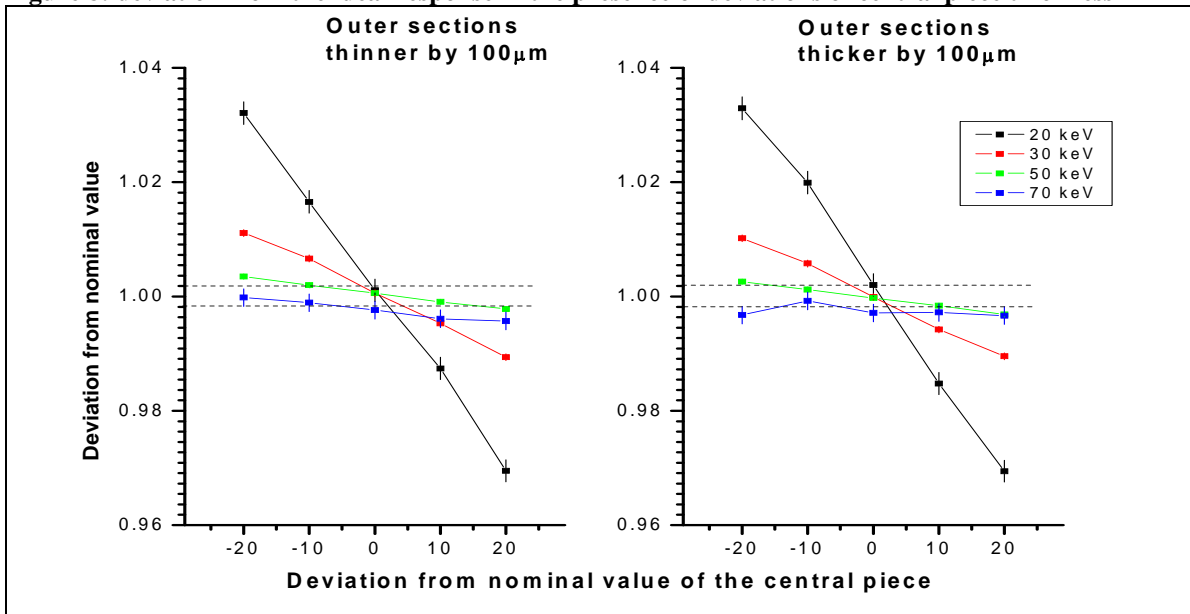
For the simulation (figure 7), the inner tube was divided in three segments, the middle one, centred on the source position, being 10 cm long. The goal of the simulation was to study to what extent achieving a very good machining accuracy for the central piece can compensate for having the other two pieces machined to very bad accuracy. Of course, the number of possibilities that can be studied is enormous (with both the outer pieces being thicker or thinner than the nominal value), so only two scenarios were chosen: the outer sections have the same thickness, which is higher or lower from the nominal value by 100 μm. For the central piece five thicknesses were considered: the nominal value, thicker by 10 or 20 μm or thinner by 10 or 20 μm.

**Figure 7: possible scenarios for the tolerances if the inner tube is made of three sections**



The results of the simulation are presented in the figure below, where the normalisation is done to a inner tube at nominal values. The dashed lines represent the acceptable variation in response that has to be achieved in the project.

**Figure 8: deviation from the ideal response in the presence of deviations of central piece thickness**



It can be seen that the predominant factor in the deviation from the response of the "ideal" inner wall can be traced to the variation of the central section. Also, it appears that the tolerance that needs to be achieved for this case is of a few micrometers, basically the same that needs to be achieved by the whole inner wall, in the hypothesis that it is made of a single piece.

While the machining complexity is reduced, in that only the central piece needs to be machined with a very good tolerance, this approach adds complexity in the required technologies to weld together the three tubes so that they are both leak-tight and structurally sound. Additional issues might arise from the alignment of the three components during/after the welding procedure.

### 3.3 Study of the influence of the material composition for the inner wall of the IC

Since the start of the project it was clear that the materials that are used for the construction of the ionisation chamber have to be specified in the project, but no actual study was performed so far concerning the level of detail of this specifications. The study presented in this section approach the issue of the material used for the construction of the inner wall of the ionisation chamber.

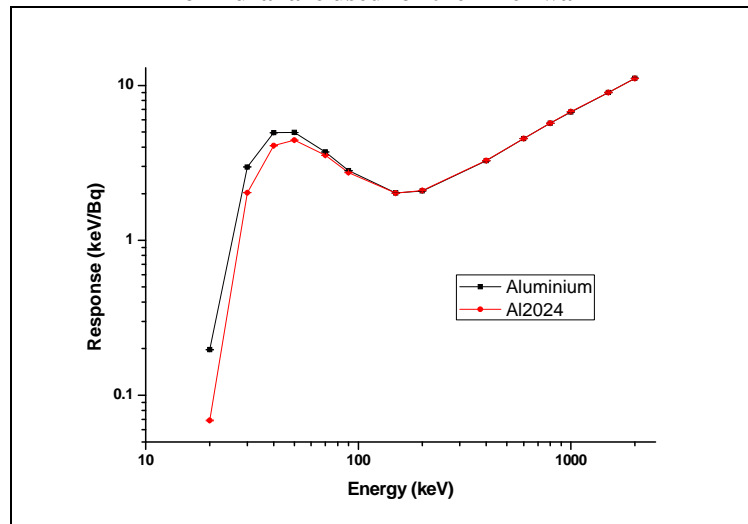
Dural and Aluminium are the most obvious candidates for the construction of the inner wall of the ionisation chamber because of the low self-absorption (low Z), mechanical and machining properties. Nevertheless, Dural is a generic name for a whole class of Aluminium alloys (Al2024) for which the impurities are defined in a rather broad range, especially if we think of the required 0.2% accepted variation for the response required by the project.

The table bellow presents a version of the accepted composition of the Al2024 alloy:

Alloy	Si (%)	Fe (%)	Cu (%)	Mn (%)	Mg (%)	Cr (%)	Zn (%)	Ti (%)	Al
2024	0.50	0.50	3.8-4.9	0.3-0.9	1.2-1.8	0.1	0.25	0.15	Rest

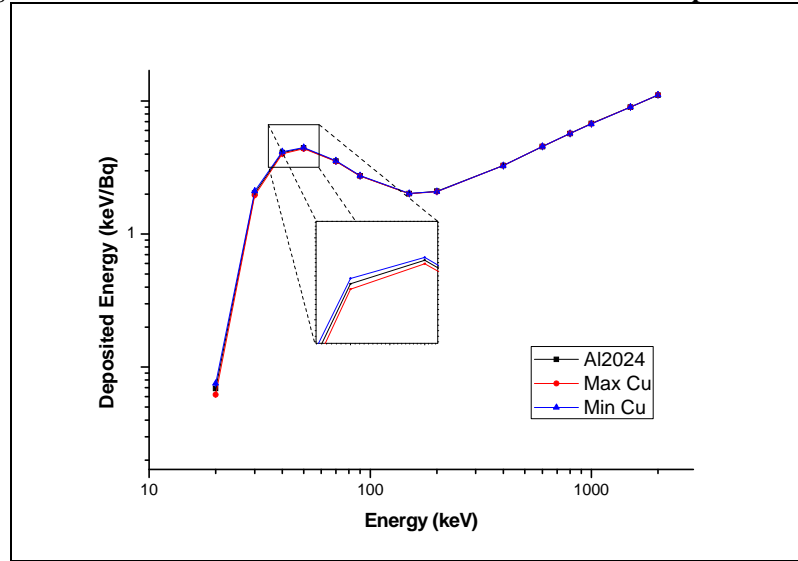
Simulations were performed, where the only variation was the composition of the inner tube. At first, the difference between using pure Al and the "average" Dural alloy was studied. It is clear from the figure bellow that the difference in response is significant at energies lower than 100 keV.

Figure 9: comparison of the response for the cases where Aluminium or Dural are used for the inner wall



The following figure presents the variation of the response when the maximum and minimum Cu concentrations are compared to the "average" values. (Note: the variation of concentration on one of the components is compensated by a variation of the Al concentration). It is obvious that there are differences, but this type of graphical comparison is lacking because of the small differences in response.

**Figure 10: influence of the Cu concentration in Dural on the response**

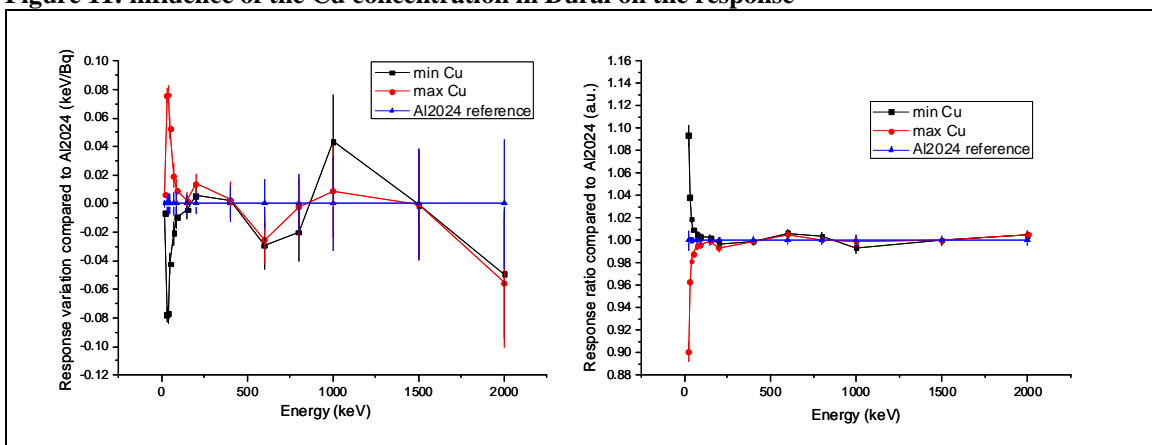


To better compare the results, two types of graphs are employed: one, where we compare the difference between the response for different concentrations and the "average" concentration to get an idea of the amplitude of the variation. In a second analysis we compare the relative variation with the goal to obtain an assessment of the impact on the response, relative to the 0.2% required by the project objectives.

The effect of Cu, Mn and Mg were studied because, according to the "definition" of Al2024, these are the impurities most likely to vary across different batches of Dural.

**Effect of Cu:** the variation on Cu concentration becomes important below 100 keV, because of the relative high Z-value of Cu. The variation of the Cu concentration has, at these energies, an impact much higher than the 0.2% reproducibility goals of the project. It can be seen that at 20 keV a variation of 1% in the Cu concentration can lead to a 10% variation of the response at 30 keV. This means that the concentration of Cu in the material used for the inner wall needs to be known to a very good accuracy.

**Figure 11: influence of the Cu concentration in Dural on the response**

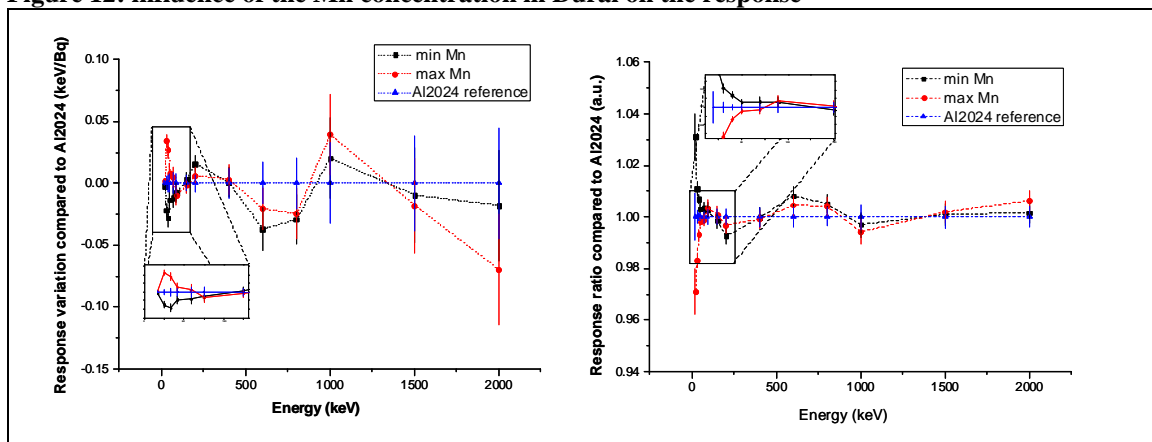


**Effect of Mn:** the impact of the variation of the Mn concentration becomes clear only at energies lower than 50 keV, and goes above the specifications only at 30 keV, which



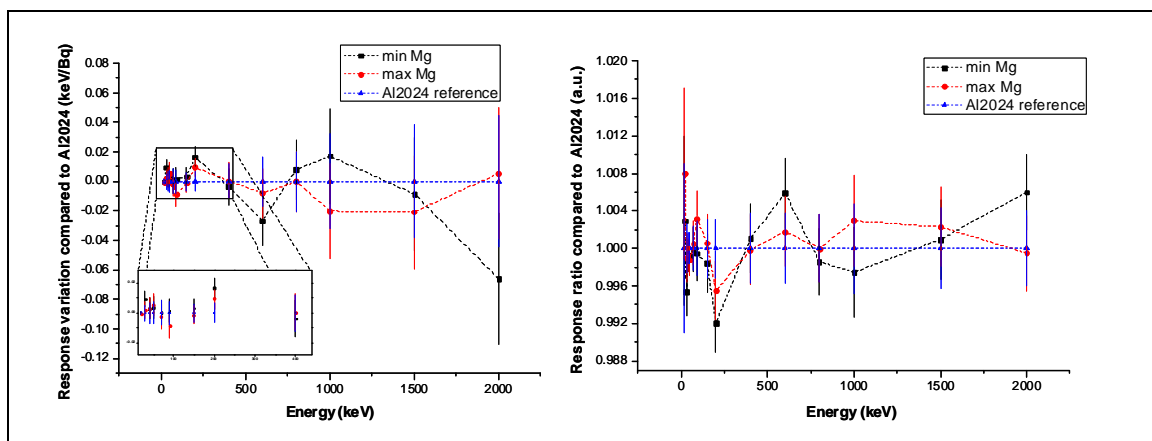
means that while care should be taken about the concentration of Mn in the material, it is not as critical as the the concentration of Cu.

**Figure 12: influence of the Mn concentration in Dural on the response**



**Effect of Mg:** no effect due to the variation of the Mg concentration can be seen.

**Figure 13: influence of the Mg concentration in Dural on the response**



In conclusion, the composition of the material used for the inner tube of the ionisation chamber should be taken into account when two or more chambers are built at different times, with Dural obtained from different producers.

### 3.4 Simulations supporting the new prototype

In 2010 the discussions on a new prototype were started. The main differences compared to the previous prototype come from the addition of two additional electrodes (together with their guard rings) that have a double role: to separate the structural properties of the chamber from the electrical ones (so that the inner wall plays no part in the charge collection) and to define more precisely the charge collection volume.

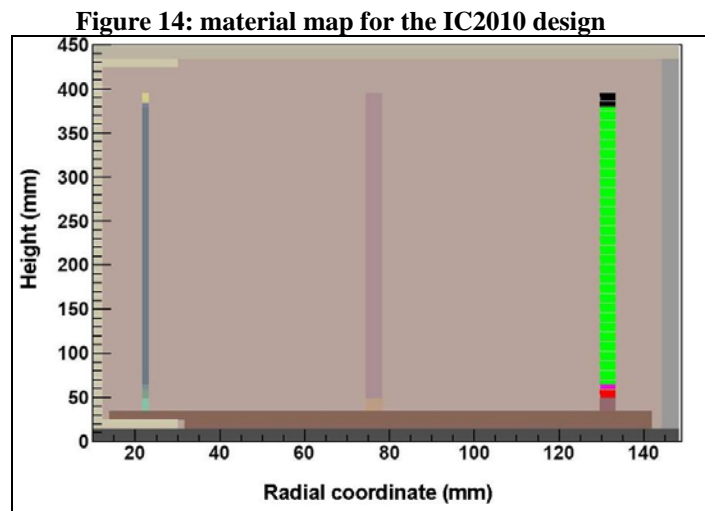
The following sections describe the investigations of these claimed benefits of the new prototype using the Monte-Carlo code.

### 3.4.1 Study of the importance of the charge collection on the response

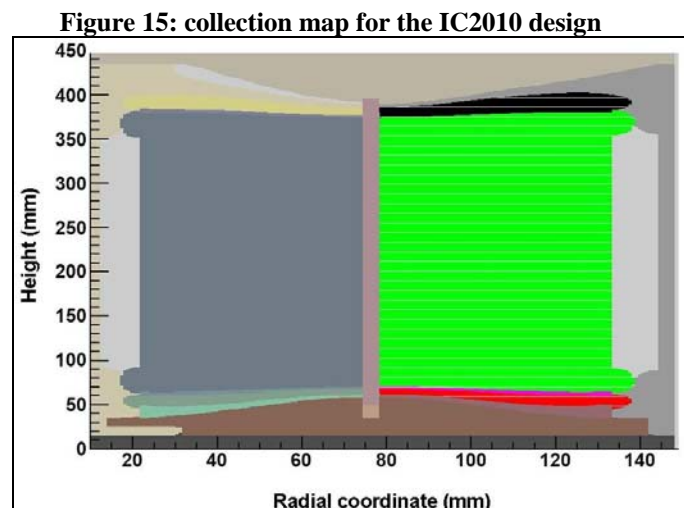
The charge collection is expected to play an important role in the fulfilling the requirements for the variation of the response because the new prototype has a number of "dead" volumes, from which the deposited charge in gas is not collected.

The ingredients of the charge collection algorithm are presented bellow:

- the material map displays, on the grid obtained from ELMER, the distribution of materials in the chamber (in figure 14 each material being represented with a different color).

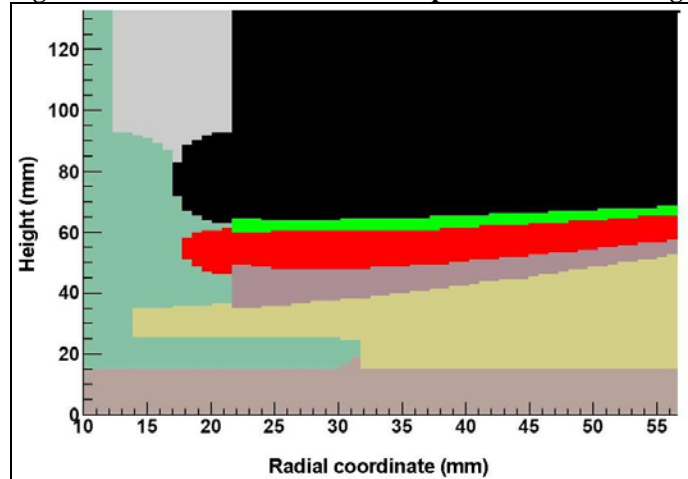


- the charge collection map, describes which of the components collects the charge deposited in the gas. It can be seen, for example, that the most of the charge deposited in the gas is collected by the two electrodes.



The collection volume is clearly defined, but trouble zones can be identified: the lobes "behind" the electrode and the zone corresponding to the insulator between the electrode and the ring.

**Figure 16: detail on the collection map for the IC2010 design**

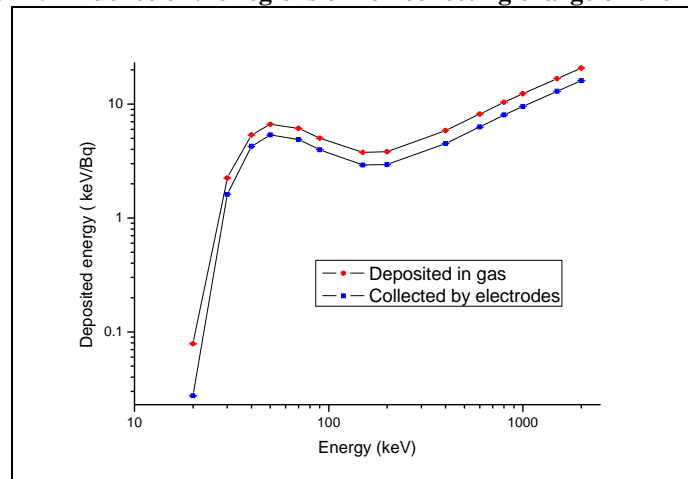


Another purpose of the charge collection map is to assess the importance of the zones with uncertain charge collection, such as the areas behind the electrodes (where the field is very low, but some field lines "creep in" through the distance separating the electrodes from the guard rings) as well as the zone corresponding to the separation between the electrodes and the guard ring, where part of the charge is collected by the electrode and the rest by the guard ring (visible in red in the third picture, showing a detail around the guard ring). The volume shown in green represents the volume where the collection is uncertain, and gives an estimate of the precision of defining the collection volume for the new design.

Results of the simulation:

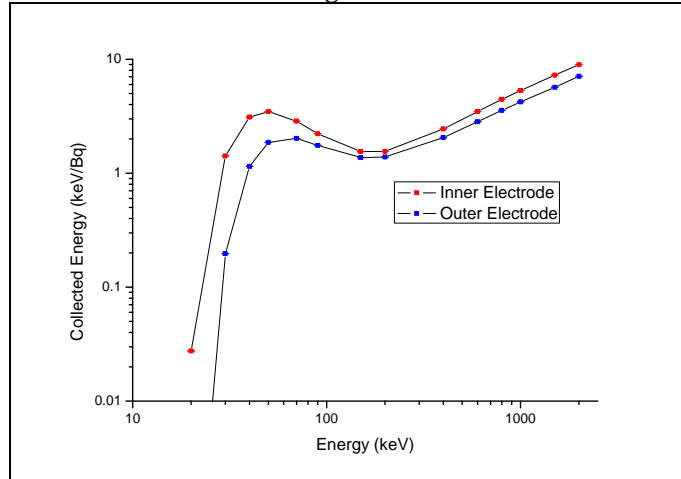
1. the collection of charges does matter significantly, so for estimating the response of the prototype a simulation (or any other type of calculation) must have a way to describe the areas from which the charge is collected.

**Figure 17: influence of the regions of non collecting charge on the response**



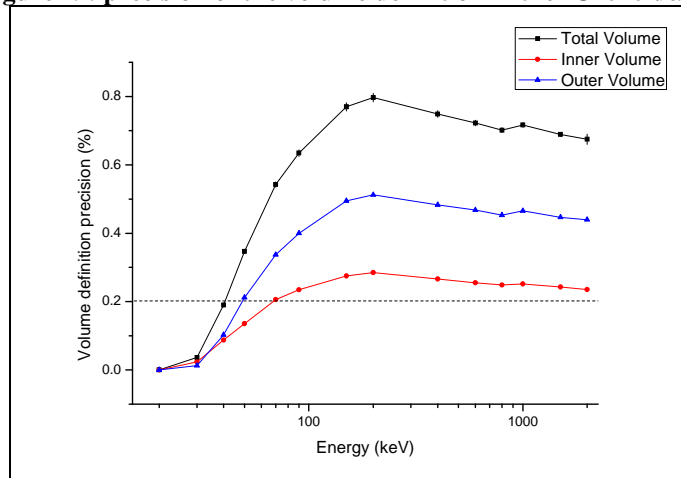
2. the distribution of collected charge between the two electrodes: the first electrode collects always more charge than the second. This unequal distribution of the current between the two electrodes should be taken into account when the electrical circuits for reading the chamber signal are designed

**Figure 18: distribution of the charge collected between the two electrodes**



3. the insulators separating the guard rings seem appropriate, but as a design goal, they should be as small as possible. The graph below shows the total charge in the non-collection volume between the collecting electrodes and the neighbouring guard rings. In reality, the error on the sensitive volume will be given by only a fraction of that volume. Additionally, in the simulation, the separation between the guard ring and electrodes was taken as 5 mm, which could be made smaller in the prototype. An additional observation is that for the purpose of defining the collection volume, the insulators on the outer ring are more important than those on the inner ring.

**Figure 19: precision of the volume definition in the IC2010 design**

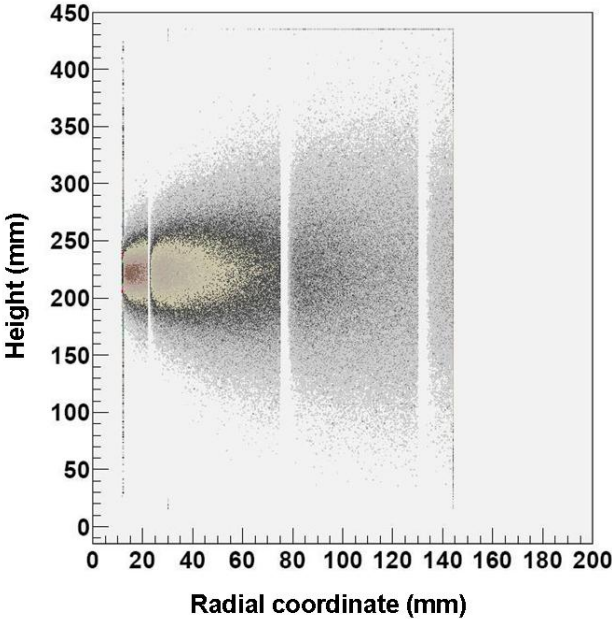


### 3.4.2 Two dimensional maps of the deposited/collected energy

Two dimensional maps of the deposited/collected energy were added to the simulation to investigate the volume definition asymmetry described above and proved a very useful supplemental test that the simulation is performing as expected. The figures below present the energy deposited in the gas for a cylindrical source (ampoule) emitting 1MeV photons. It can be seen that most of the energy is deposited around the centre of the chamber, diminishing the effects of the trouble spaces (the lobes at the end of the electrode and the volume corresponding to the distance between the electrode and the guard rings for the inner ring) on the response.

Of high interest for the project is the non-collected volume between the inner wall and the first collecting electrode, where a significant charge is deposited.

Figure 20: charge deposited in gas in IC2010 design



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## Additional information

### Appendix 1: The configuration file

additional information for running the simulation	1.	Comment line
1	2.	run mode
ICsource.inp	3.	Source description filename
IC2010.inp	4.	Geometry description filename
ICanalysis.inp	5.	Analysis description filename
0.01	6.	cut-off value (mm)
vis.mac	7.	default visualisation macro
CollectionMap.dat	8.	collection map filename
5	9.	id of the gas in the collection map
1	10.	turn charge collection on (1)/off (0)
1 5 2 10 18	11.	gas collection parameters
case.ep	12.	elmer fields file
matMap.dat	13.	material map file

The left side presents an example of configuration file. The right side is a brief description of the field. Additional information on these can be found below.

#### 1. Comment line

Can be any line of text. Can be used to describe in input file

#### 2. run mode

Used to select the purpose of the simulation.

runMode=

1 : the normal simulation run; calculates "ICresults.root"

2 : visualisation of the geometry; execution deferred to the visualisation macro

3 : create the material map file (from the FEM-Elmer file and geometry)

4 : create the charge collection map file (from the FEM-Elmer file, the geometry and materials map)

#### 3. Source description filename

#### 4. Geometry description filename

#### 5. Analysis description filename

#### 6. cut-off value (mm)

#### 7. default visualisation macro

#### 8. collection map filename

#### 9. id of the gas in the collection map

#### 10. turn charge collection on (1)/off (0)

#### 11. gas collection parameters

id of the gas volumes in the Geant4 simulation and of the collection electrodes; format:

noOfGasVolumes listOfGasVolumes noOfCollectionElectrodes listOfCollectionElectroded

Example: a single gas volume (noOfGasVolumes=1) is used, the gas is the piece number 4 in the geometry; there are two collection electrodes, bearing number 10 and 18 in the geometry file

#### 12. Elmer fields file

#### 13. material map file

## Appendix 2: Particle source file

```

source description in a few words: random photons from a
vial;
2
0 0 21.825 0 0.7645 1.0 0 0 0 0
14
4 55137 10000000
.....
4 53125 10000000

```

1. Comment line
2. shape of the source
3. parameters for the source shape
4. number of radionuclides
5. radionuclide 1
6. ....
7. radionuclide n

The left side presents an example of source configuration file. The right side is a brief description of the field. Additional information on these can be found bellow.

1. Comment line
2. shape of the source
  - 1: point source:
    - parameters:
      - position: x(cm), y(cm), z(cm)
  - 2: uniform distribution in a cylinder:
    - parameters:
      - position: x(cm), y(cm), z(cm)
      - size: innerRad(cm), thickness(cm), halfLenght(cm)
3. parameters for the source shape: 15 values are expected;
4. number of radionuclides
5. radionuclide 1 :
  - a. radionuclide code:
    1. (gamma) energy (keV) activity (number to be simulated)
    2. (e- =  $\beta^-$ ) energy (keV) activity filename
    3. (e+ =  $\beta^+$ ) energy (keV) activity filename
    4. radionuclide ZZAAA activity  
(Z and A are used to find the file zZZaAAA.dat)
    5. (e- = conversion electron) energy(keV) activity



### Appendix 3: Analysis file

```
analysis description in a few words
1000000
0
24
1 1000 0 200
  1000 -15 450
  1000 -180 180
2 1000 0 200
  1000 -15 450
  1000 -180 180
.....
24 1000 0 200
  1000 -15 450
  1000 -180 180
```

1. Comment line
2. No of intermediate events
3. TreeOutput
4. number of histograms
5. objId nrBinsR lowBinR highBinR
6. nrBinsZ lowBinZ highBinZ
7. nrBinsPhi lowBinPhi highBinPhi
8. ....

The left side presents an example of analysis configuration file. The right side is a brief description of the field. Additional information on these can be found bellow.

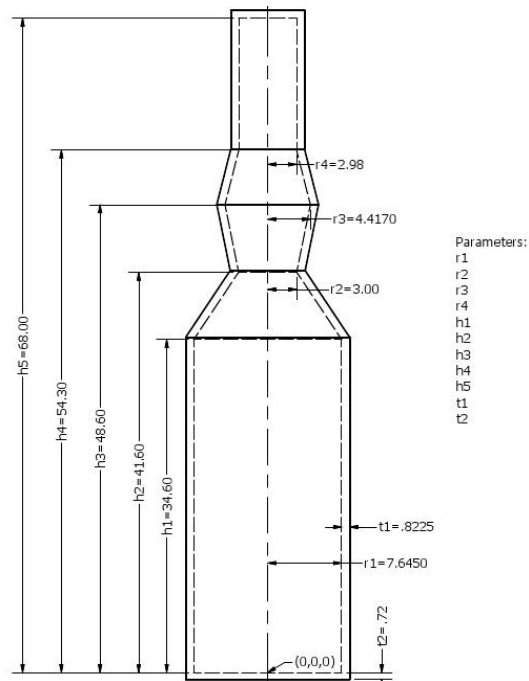
1. Comment line
2. No of intermediate events: used for calculating the intermediate values, errors...
3. TreeOutput On(1)/Off(0)
4. number of histograms: how many histograms are being modified
5. objId nrBinsR lowBinR highBinR : the objId that has it's histogram modified and the new ranges for (R,Z,Phi)



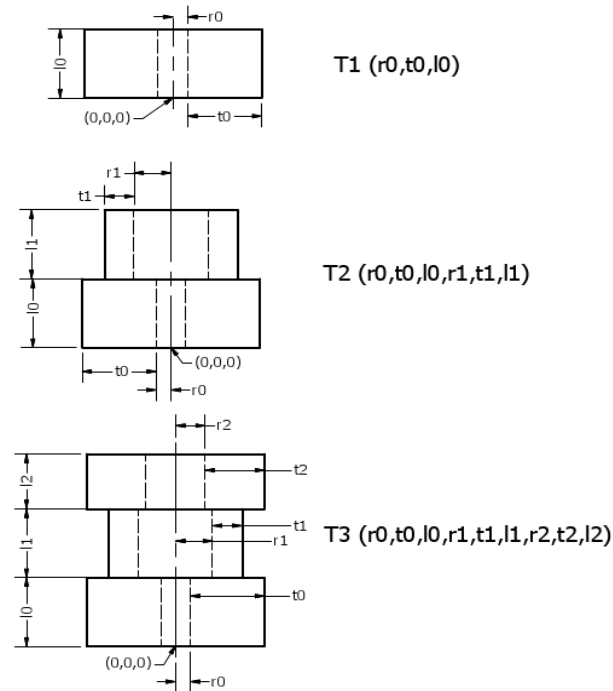
## The shape codes

The shape codes (shapeID) are the codes of the building blocks making up the structure of the ionisation chamber. The meaning of the shape codes can be found bellow.

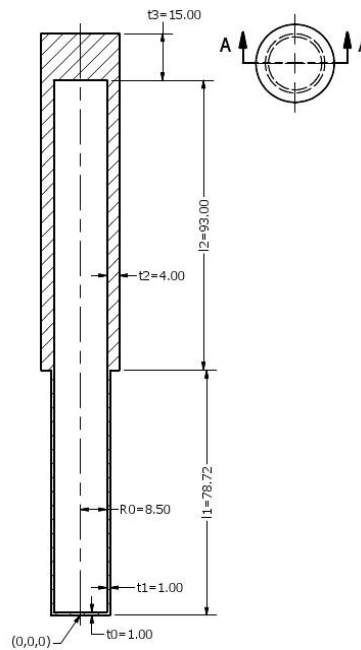
1. Box: shapeID= 1; parameters: halfLenghtX(cm), halfLenghtY(cm), halfLenghtZ(cm);
2. source ampoule
  - a. shapeID= 21 shape 1 (flat bottom, straight neck):
  - b. shapeID= 22 shape 2 (flat bottom, shaped neck, neck dimensions relative to the other dimensions)
  - c. shapeID= 23 shape 3 (taken from J.Champs MCNP simulations)



2. Tube: 3 types of tube have been implemented: 31 - T1, 32 - T2, 33 - T3



3. source holder  
a. shapeID=41



**Materials**

The materials used by the existing prototype or expected to be used by the prototype were hardcoded in the simulation. On top of those, the NIST materials database can be used (for example G4\_WATER denotes water, as described by NIST).

## **Sensitive components**

Geant4 allows a separation between the structural components and the sensitive ones. The sensitive components are those whose interactions are being analysed.

This parameter is set to 1 if the component is active for detection, and 0 if it is a structural component.

In a real ionisation chamber the only sensitive component is the pressurised gas, but the simulation allows the study of energy loss in each of the components. In the example, all the components are declared as sensitive, so that the energy loss in each of them can be studied.

## **RGB code and visualisation**

Geant4 allows the rendering of the geometry of the detector on a number of graphic interfaces for the purpose of "debugging" the geometry. This 3D representation becomes complicated when all the components are visible, so switches were implemented to toggle the visibility of the different objects. The 9 digits RGB colour code sets the colour that the object will have in the representation (RRRGGBBB).

## Appendix 5: Precision of the simulation

Calculating the energy deposited in each component is only the first step in obtaining meaningful results from the Monte Carlo simulation. The Geant4 framework does not supply the means to analyse the accuracy and precision of the energy deposits, but provides an easy mean for them to be developed by the user, as part of the analysis. In this respect, the strength of the Geant4 framework lies in that it gives full access to the information about each hit in the detector.

Notations:

- detector: one sensitive component in the Geant4 geometry
- $x_i$  is the energy deposited in one detector during an event (During each event, there might be more interactions in the same detector, depending on the complexity of the event/detector. If this is the case,  $x_i$  is the sum of these energy deposits)
- N is the number of events that were simulated
- $S_j = \sum(x_i)^j$  are the sums of the different energy depositions, updated after each event.

With these notations, the following values are calculated:

- Mean =  $S_1/N$  : the mean energy deposited during one event
- SDev =  $\sqrt{S_2/N - \text{Mean}^2}$  : the standard deviation of the energy deposits during one event
- MeanSDev =  $\text{SDev}^2/N$  : the standard deviation of the mean
- RelErr = MeanSDev/Mean : the relative error of the mean
- VoV =  $(S_4 - 4S_1S_2/N + 8S_2S_1^2/N - 4S_1^4/N^3 - S_2^2/N) / (S_2 - S_1^2/N)^2$  : the variance of variance

In principle, these values can be calculated (and saved) after each event, but this would generate a very high amount of (useless) information, if we are taking into account that the number of events in a simulation is of the order of  $10^6$ . To bypass that, a parameter was included in the analysis configuration file of the simulation that decides how often this value to be calculated and saved. They are always calculated at the end of the simulation.

Note: these precision estimates are replicating the method used by MCNP and described in chapter IV of the manual: "Estimation of the Monte Carlo precision"

## Appendix 6: Charge collection

Simulating the charge collection in the ionisation chamber requires the knowledge of the (stationary) electrical fields that are present when the chamber is in operation, the knowledge of where the interaction takes place (starting point for the movement of charges) and a possibility to check, after each of the iterative steps if the charged particle has reached the boundary of the gas. In principle, none of these steps is performed using the Monte-Carlo method, but nonetheless, performing the charge collection as part of the simulation has clear advantages: the start point of the track is generated by the simulation, and the geometry can be interrogated to decide if the charge cloud has reached the boundary. Tracking is performed assuming that all the charge cloud moves through the gas a single particle.

In practical terms the following steps are to be followed to implement the charge collection:

1. define the geometry of the chamber
2. identify the 2D part that is to be used in the fields calculation
3. run the fields calculation using ELMER
4. run the simulation to create the materials map ( interrogates the Geant4 geometry about what object contains each of the fields grid nodes)
5. run the simulation to create the collection map (an optimisation step; most of the space in the collection volume will be collected by the electrodes, so at this point for each node of the grid a charge is created and tracked; the cells where the adjacent nodes are collected by the same electrode will be collected by the same electrode)
6. run the simulation (only the interaction points at "difficult" positions according to the collection map are tracked, the rest are taken from the collection map).

Notes on the implementation:

- the grid used in ELMER must be rectangular
- the fields inside the cells are calculated by bilinear interpolation
- the charges are propagated from interaction to first intersection with the grid, then from grid line to grid line
- the collection is stopped when either the charge takes too long to be collected (is in a low field area) or when it exits the gas;





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## Abstract

Monte Carlo simulations have become an integral part of developing new radiation detectors and the work on the ionisation chamber that is being built as part of the project "Realisation of the Bq" makes no exception. Until now, Monte Carlo simulations were performed at IRMM using EGS4 and MCNP5 and at LNHB using Penelope. Some of these simulations were used to define the parameters of a prototype ionisation chamber, while others dealt with other aspects of the operation of the chamber such as the effect of the ampoules holding the source, or the positioning of the ampoule. In 2010 the work started on designing a new prototype. At the same time, a new simulation program for the project was started, using the Geant4 framework.

This technical document presents the details of the simulations as they were performed using the Geant4 framework, focusing on the last version of the simulation code. This document, together with the source code and the documentation included in the source code should provide enough information for anyone to reproduce the results and expand the simulations.

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