



HAL
open science

A benchmark for Monte Carlo simulation in gamma-ray spectrometry

Marie-Christine Lépy, Cheick Thiam, M. Anagnostakis, R. Galea, D. Gurau, S. Hurtado, K. Karfopoulos, J. Liang, H. Liu, A. Luca, et al.

► **To cite this version:**

Marie-Christine Lépy, Cheick Thiam, M. Anagnostakis, R. Galea, D. Gurau, et al.. A benchmark for Monte Carlo simulation in gamma-ray spectrometry. *Applied Radiation and Isotopes*, 2019, 154, pp.108850. 10.1016/j.apradiso.2019.108850 . cea-02475801

HAL Id: cea-02475801

<https://cea.hal.science/cea-02475801>

Submitted on 14 Feb 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

A BENCHMARK FOR MONTE CARLO SIMULATION IN GAMMA-RAY SPECTROMETRY

M.C. Lépy¹, C. Thiam¹, M. Anagnostakis², R. Galea³, D. Gurau⁴, S. Hurtado⁵, K. Karfopoulos⁶,
J. Liang⁷, H. Liu⁷, A. Luca⁴, I. Mitsios², C. Potiriadis⁶, M.I. Savva⁸; T. T. Thanh⁹, V. Thomas¹⁰,
R.W. Townson³, T. Vasilopoulou⁸, M. Zhang⁷

1: CEA, LIST, Laboratoire National Henri Becquerel (LNE-LNHB), Bât. 602 PC 111, CEA-Saclay 91191 Gif-sur-Yvette Cedex, France, 2: NED-NTU Athens, Greece, 3: NRC, Canada, 4: Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH), 30 Reactorului street, PO Box MG-6, Magurele, Ilfov county, RO-077125, 5: U. Sevilla, Spain, 6: EEA, Greece, 7: NIM, China, 8: INRASTES, NCSR "Demokritos", Greece, 9: VNUHCM-US, Vietnam 10: CEA/DAM, France

Keywords: Monte Carlo simulation, gamma-ray spectrometry, efficiency, EGS-nrc, GEANT4, GESPECOR, MCNP, PENELOPE

Highlights:

Examples of the use of Monte Carlo simulation using different software.

Simple cases with two types of germanium detectors and four kinds of sources.

Calculation of full-energy peak and total efficiencies for 5 energies.

Input files and efficiency calculation results available on a dedicated webpage.

ABSTRACT

Monte Carlo (MC) simulation is widely used in gamma-ray spectrometry, however, its implementation is not always easy and can provide erroneous results. The present action provides a benchmark for several MC software for selected cases. The examples are based on simple geometries, two types of germanium detectors and four kinds of sources, to mimic eight typical measurement conditions. The action outputs (input files and efficiency calculation

results, including practical recommendations for new users) are made available on a dedicated webpage.

1. Introduction

Monte Carlo simulation of radiation transport continues to grow in popularity in the fields of medical physics and radiation measurement, due in part to improvements of computation speed and to the modern usability of the codes. This concerns many different fields of application and, in the specific case of gamma-ray spectrometry, simulation is now commonly used to compute practical parameters which are used to quantify radioactivity in sample, such as the detection efficiency (Sima, 2012) and coincidence summing corrective factors (García-Toraño *et al.*, 2005).

Accurate efficiency calibration is required to perform optimisation procedures, by comparing the calculation results with experimental data on a large energy range, to validate the geometrical parameters used in the simulation model (Helmer *et al.*, 2004, Hurtado *et al.*, 2004, Peyres and García-Toraño, 2007).

Even if absolute detection efficiency values are difficult to calculate *ab-initio*, because of the lack of accuracy in the geometrical parameters of the detector, Monte Carlo simulation has been proved to be an efficient method to compute efficiency transfer factors such as it was demonstrated by Vidmar *et al.* (2008).

Two kinds of Monte Carlo simulation software are used in gamma-ray spectrometry: these are either general multi-purpose codes (EGS, GEANT4, MCNP, PENELOPE, etc.) or dedicated ones such as GESPECOR (Sima *et al.*, 2011), DETEFF (Cornejo Díaz and Jurado Vargas, 2008), etc. The dedicated codes are conceived with a user-friendly interface and can be directly applied to derive the calculation results from input data. On the contrary, the use of generalist codes needs some training in order to derive the information of interest. One of the typical difficulties is the preparation of the input files which specify the geometrical conditions, since these must be written with a specific format.

This can be a challenge for new users who do not benefit from the advice of experienced users. Thus, in the frame of the Gamma-Ray Spectrometry Working Group (GSWG) of the International Committee for Radionuclide Metrology (ICRM), it was suggested to provide some case studies and to prepare the corresponding input files for several codes, together with the expected results of the simulation. Comparisons between input files and results prepared by several participants should ensure reliability of these data, with final goal to make these easily and freely available for training purpose.

2. Presentation of case studies

As training to use Monte Carlo (MC) simulation software, it was proposed to prepare geometrical files for a selection of high-purity germanium detectors (HPGe) and measurement conditions. In a first step, the exercise started with the simple models which were defined by Vidmar (2014) in an exercise dedicated to coincidence summing corrections. Geometry models include a detector and a source with different combinations; however, in all the cases, complete cylindrical symmetry of the arrangement of sample and detector is assumed.

Two kinds of coaxial high-purity germanium (HPGe) detector are considered. For both, the active crystal of the detector consists of a germanium cylinder with a thickness and diameter of 60 mm, with a 40-mm depth hole of 10-mm in diameter, with relative efficiency of about 20%. It is installed in a 1-mm thick aluminium housing, with a length and diameter of 80 mm, and the crystal-to-window distance is 5 mm. The only difference between the two models is the dead layer thickness (on the top and side of the crystal), that is 1 mm or 0 mm to simulate either a p-type detector ("Detector A") or a n-type one ("Detector B").

One point source and 3 volume sources are considered, each located at 1 mm from the detector window. No source containers are to be simulated and the volume sources are cylinders made of water (Diameter 90 mm – thickness 40 mm), silicon dioxide (Diameter 60 mm – thickness 20 mm) and cellulose (Diameter 80 mm – thickness 3 mm) with respective density 1.0, 1.4 and

0.3. The last two sample models are supposed to reproduce the measuring conditions of soils and filters. These sources are respectively denoted “P”, “W”, “S” and “F” in the exercise.

Each source-detector assembly is installed in a 50-mm thick lead shielding, which has both a diameter and a height of 400 mm. The characteristics of various materials to be used in the simulation of the detector and sample models were also provided according to Vidmar (2014). On the whole, eight configurations (2 detectors X 4 sources) were to be prepared. Figure 1 shows an example of the p-type detector in combination with the water source (without the external shielding).

For each configuration, the participants were asked to prepare input files specific to the MC code they are familiar with, and to compute the full-energy peak efficiency (FEPE) and the total efficiency (TE) for five energies (50 keV, 100 keV, 200 keV, 500 keV and 1 MeV), for the eight combinations named “AP”, “AW”, “AF”, “AS”, “BP”, “BW”, “BF” and “BS”.

3. Short presentation of the Monte Carlo codes

In the present exercise, the participants used four general purpose codes (EGSnrc, GEANT, MCNP, PENELOPE) and one dedicated software (GESPECOR), and most of these have been used by several participants. We summarize hereafter the general features of each code, mainly from the point of view of a "new user" for the practical use of Monte Carlo simulations. As each code requires specific input files to carry out the calculation, the participants in the action agreed on some common parameters and, if applicable, on the preparation of the calculation input files. A summary of the main parameters used in the simulations is presented in Table 1.

3.1 EGSnrc

EGSnrc (Electron Gamma Shower) (EGS, 2019) models the propagation of photons, electrons and positrons with kinetic energies between 1 keV and 10 GeV, in homogeneous materials. It is an open source software toolkit with applications in a range of radiation-related fields, particularly medical dosimetry. EGSnrc is an extended and improved version of the EGS4 code earlier developed (Nelson et al., 1985). The EGSnrc implementation improves the accuracy and precision of the charged particle transport mechanics and the atomic scattering cross-section data (Kawrakow, I., 2000), and includes a C++ class library for defining the geometry of complex simulation environments and particle sources. The core EGSnrc transport code remains in the Mortran language (Cook, 1983) which is an extended Fortran. For most applications, users can specify complex simulations using input files, without the need to write code. Visualization tools and GUIs are included.

3.2 GEANT4

GEANT4 (GEANT4, 2019) (GEometry ANd Tracking) is a general purpose Monte Carlo toolkit for the simulation of the passage and interaction of particles through matter, developed at CERN (Agostinelli *et al.*, 2003, Allison *et al.*, 2006, Allison *et al.*, 2016). It is written in C++ and exploits advanced software-engineering techniques and object-oriented technology. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. GEANT4 offers a set of functionalities defined in specific C++ classes which users can call on to describe the different aspects of the experiment simulation (geometry, physical processes governing particles interactions, visualization of the detector and particle trajectories, data analysis at different levels of detail, etc.). However, the user must build his own application with tree mandatory classes: *MyDetectorConstruction* class, in which the geometry is defined in terms of volumes and filling materials physical properties; *ExpDetectorConstruction* class, in which particles, interaction processes and physical models

are specified through *ExpPhysicsList* class; and *ExpPrimaryGenerator* class in which the generation of primary particles is defined in *MyPrimaryGenerator* class. Optional classes can be added to manage the simulation stages when its progresses (*MyRunAction*, *MyEventAction* and *MySteppingAction* etc.). A main program permits to run the simulation by calling in turn and bringing together the set off the basic and user Geant4 classes.

3.3 GESPECOR

GESPECOR (Germanium SPectra CORrection) is a Monte Carlo based software, dedicated to gamma-ray spectrometry providing practical tools to perform the calculation of corrective factors (efficiency transfer, self-attenuation and coincidence summing corrections) and based on the methods developed by Sima et al. (2001). The computation routines are launched through a user-friendly interface, which can directly be applied to coaxial, planar or well-type high-purity germanium (HPGe) detectors with realistic dimensions including bulletized crystal, in a wide range of measurement configurations. Initially developed for the computation of the self-attenuation corrections and of the coincidence-summing corrections required to provide accurate quantitative results in gamma-ray spectrometry, the computation of the full energy peak efficiency and of the total efficiency was later added. Due to the optimization of the procedure, GESPECOR provides results in a fast time. Comparisons of the results obtained by GESPECOR and GEANT have been published (Chirosca *et al.*, 2013). GESPECOR version 4.2 was used by two participants.

3.4 MCNP

MCNP6 (MCNP, 2019) in the newest version of is the general-purpose Monte Carlo N-Particle code, developed at Los Alamos National Laboratory, that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport (Briesmeister *et al.*, 2000, Goorley *et al.*, 2013). Specific areas of application include radiation protection and dosimetry, medical

physics, nuclear criticality safety, etc. The code is written in Fortran and the user sets up simulations by creating a text file that is read by MCNP6. This input file has a dedicated structure and includes the geometry definition, and every information needed for the radiation transport for the specific problem (source, materials, type of answers or tallies desired and any variance reduction techniques used to improve efficiency). A dedicated visualization tool (<http://www.mcnpvised.com/visualeditor/visualeditor.html>) allows checking the geometry definition.

3.5 PENELOPE

PENELOPE, an acronym for "PENetration and ENergy LOss of Positrons and Electrons" is developed by the University of Barcelona and was initially dedicated to the transport of electrons and positrons in the matter. Since then, it has been completed by the addition of photon transport, for an energy range from 100 eV to 1 GeV (Salvat, 2015, Salvat and Fernández-Varea, 2009). PENELOPE is programmed in FORTRAN77 and can be started by two predefined main programs: PENCYL or PENMAIN. The main difference between these is that the geometry of PENCYL is only cylindrical while PENMAIN allows a more complete set of three-dimensional surfaces to be used. The simulation details and the geometry are described in two separate files: the input file, with the extension ".in", includes the information about the source, materials and geometry characteristics, the requested output files and the simulation conditions, and the one with the extension ".geo" contains the geometrical model. In the recent release of the code, a graphical user Interface, PenGeomJar, developed under Java facilitates geometry preparation and its two- and three-dimensional viewing.

4. Results and discussion

The exercise was carried out by 11 participants who provided nineteen sets of results, some participants using different versions or options of the same software or running different codes.

Figures 3-a and 3-b display the FEP and total efficiency values for detector A and B respectively, each result being obtained as the mean value of initial nineteen data sets provided by the participants. The standard deviation is used to plot the associated uncertainty bars. As seen in Figure 3, the standard deviation of each set of results is rather high, especially for the total efficiency. Thus, a more detailed analysis of the use of each code was performed to understand the causes of the discrepancies in order to reduce these when new calculation were carried out in a second step.

Tables 2-6 summarize the numerical results, quoted by code, with the mean value and the standard deviation for each case.

When examining into details Tables 2-6 and the individual results, some discrepancies or systematic deviation were noted; as a results of a complementary analysis, most of these could be understood and reduced to provide the final set of results. Some of these complementary investigations are developed hereafter:

1. In a first step, small discrepancies between the GEANT4 participants results were noted, and it was supposed that this could be due to the difference between the electromagnetic (EM) physics that is used in the simulation, since there are four EM physics model available in GEANT:

"emstandard"	standard EM physics with current 'best' options setting,
"emlivermore"	low-energy EM physics using Livermore data,
"emlowenergy"	low-energy EM physics implementing experimental low-energy models,
"empenelope"	low-energy EM physics implementing PENELOPE models.

To clarify, complementary calculations were run with the four options, by the same participant. A summary of these results is presented in Figure 4 for detector A and the point source, where

“ D_i ” is plotted for each physics model (i), as the quadratic sum of the relative differences for the five energies, computed as:

$$D_i = \sum_E \left(\frac{FEPE(E) - M(E)}{M(E)} \cdot 100 \right)^2 \quad (E = 50 \text{ keV}, 100 \text{ keV}, 200 \text{ keV}, 500 \text{ keV}, 1000 \text{ keV})$$

and

$$M(E) = \frac{\sum_i FEPE(E)}{4}$$

This clearly demonstrated that the “emstandard” and “empenelope” models provide slightly different results than those obtained with the two other options. In the final table, the results are those obtained with the “empenelope” option.

2. Two participants reported results obtained with the dedicated software GESPECOR. Both participants used version 4.2, with software files from 2007 and 2014; very high relative differences (up to 65 %) were obtained between the two sets of results for the FEPE at 50 keV, for all the four types of samples and especially for the detector A. An update of the files used by one of the participants allowed obtaining two sets of results in good agreement. This demonstrate the necessity to carefully check the software version and associated files when performing simulations. However, comparing the results in Tables 2-6, it is obvious that all full energy peak efficiencies calculated with GESPECOR are lower than those calculated with the other codes. This might be caused by the default definition of the peak efficiency adopted in GESPECOR which is based on the definition of the peak area as the number of counts in the region delimited at the left and right of the peak by the channels with the number of counts equal to 1/10 from the peak maximum. In this case the peak area is only a factor of 0.968 from the peak area obtained by fitting a Gaussian.

3. For MCNP which was used by four participants, rather large deviation for the TE calculations were stated, and only two results (from more experienced users) were used to calculate the final mean value for the total efficiency. It was checked that the selection of the energy bin width slightly influences the results, according to the comparison of runs carried out with 1 keV and 2 keV energy bin. In addition, one participant provided two series of results calculated with and without shielding. The influence of the shielding is noticeable, especially for the low energy (50 keV) and the “light” sources (point and filter) as show in Figure 5 in the case of the point and filter sources for detector A.

4. Six participants used PENELOPE, with versions 2011, 2014 and 2016. One participant ran the PENCYL option which simplifies the geometry description in the case of coaxial cylindrical geometry, while the others used PENMAIN. The results are fairly homogeneous: for both the TE and the FEP efficiencies, the relative standard deviation of individual results is less than 1 % in all cases considered. This agreement was obtained after careful checking of the input files: indeed, it was found that the geometry of the volume source, that must be included in a “box”, can provided dramatically erroneous results, if the dimensions of “box” are not well adapted.

5. Summary and conclusion

Finally, to summarize, Table 7 shows the mean values obtained after checking of the results and rejection of a few discrepant data. Comparing the results of the different codes, one can notice some discrepancies, especially for the 50-keV incident photons. As already highlighted in a previous exercise conducted in the frame of the ICRM GSWG (Vidmar et al., 2008), there are different approaches either in the implementation of the physical interaction processes or in the practical definition of the efficiencies which prevent from achieving full comparison

between the Monte Carlo codes. However, in most of the study cases presented here, the relative standard deviation is less than 1 %.

The goal of the present exercise was to provide some practical examples for new users, what was effectively achieved. The input files for each code and the eight study cases were prepared and agreed by different users. In the same way, the calculation results, including the mean value and associated standard deviation are available. In addition, specific advices and warning to properly run the codes were derived from the experience of the users. Finally, this practical material will be distributed through the ICRM GSWG web page, so that new users may train themselves.

References

- Agostinelli S., *et al.*, 2003. GEANT4-a simulation toolkit, Nuclear Instruments and Methods A 506, 250-303.
- Allison J., *et al.*, 2006. Geant4 developments and applications, IEEE Trans. Nucl. Sci., 53, 270-278.
- Allison, J., *et al.*, 2016. Recent developments in Geant4. Nuclear Instruments and Methods in Phys. Res. A835, 186-225. (<https://doi.org/10.1016/j.nima.2016.06.125>)
- Briesmeister J.C., (Ed.), 2000. MCNP-A General Monte Carlo N-Particle Transport Code, Version 4C. Los Alamos National Laboratory Report LA-13709-M, Los Alamos.
- Chirosca, A., Suvaila, R., Sima, O., 2013. Monte Carlo simulation by GEANT 4 and GESPECOR of in situ gamma-ray spectrometry measurements, Applied Radiation and Isotopes 81, 87-91.
- Cook, A. J., 1983. Mortran3 user's guide. SLAC Computation Research Group Report CGTM-209.
- Cornejo Díaz, N., Jurado Vargas, M., 2008. DETEFF: An improved Monte Carlo computer program for evaluating the efficiency in coaxial gamma-ray detectors, Nuclear Instruments and Methods in Physics Research A, 586, 204-210.
- EGS, 2019. <http://nrc-cnrc.github.io/EGSnrc/>
- GEANT4, 2019. <http://geant4.web.cern.ch/>
- Goorley, J.T. *et al.*, 2013. Initial MCNP6 Release Overview - MCNP6 version 1.0 - LA-UR-13-22934.
- Helmer, R. G., Nica, N., Hardy, J. C., Jacob, V. E., 2004. Precise efficiency calibration of an HPGe detector up to 3.5 MeV, with measurements and Monte Carlo calculations Applied Radiation and Isotopes 60, 173-177.

Hurtado, S., García-Leon, M., García-Tenorio, R., 2004. GEANT4 code for simulation of a germanium gamma-ray detector and its application to efficiency calibration. *Nuclear Instruments and Methods A* 518, 764-774.

MCNP, 2019. <https://mcnp.lanl.gov/>

Peyres, V., García-Toraño, E., 2007. Efficiency calibration of an extended-range Ge detector by a detailed Monte Carlo simulation, *Nuclear Instruments and Methods in Physics Research A* 580, 296-298.

García-Toraño, E., Pozuelo, M., Salvat, F., 2005. Monte Carlo calculations of coincidence-summing corrections for volume sources in gamma-ray spectrometry with Ge detectors. *Nuclear Instruments and Methods in Physics Research A* 544, 577-583.

Kawrakow, I., 2000. Accurate condensed history Monte Carlo simulation of electron transport. I. EGSnrc, the new EGS4 version. *Medical physics* 27, 485-498.

Nelson, W. R., Hirayama, H., Rogers, D. W. O., 1985. The EGS4 code system, Report SLAC-265.

Salvat, F., 2015. PENELOPE-2014: A code System for Monte Carlo Simulation of Electron and Photon Transport, OECD/NEA Data Bank, NEA/NSC/DOC(2015)3. Issy-les-Moulineaux, France. Available from (<http://www.nea.fr/lists/penelope.html>)

Salvat, F., Fernández-Varea, J. M., 2009. Overview of physical interaction models for photon and electron transport used in Monte Carlo codes. *Metrologia* 46, S112–S138.

Sima, O., Arnold, D., Dovlete, C., 2001. GESPECOR – a versatile tool in gamma-ray spectrometry. *Journal of Radioanalytical and Nuclear Chemistry* 248, 359-364.

Sima, O., 2012. Efficiency calculation of gamma detectors by Monte Carlo methods, in *Encyclopedia of Analytical Chemistry*, Online, Wiley

Vidmar, T., Aubineau-Lanière, I., Anagnostakis, M., Arnold, D., Brettner-Messler, R., Budjas, D., Capogni, M., Dias, M.S., De-Geer, L.-E., Fazio, A., Gasparro, J., Hult, M., Hurtado, S.,

Jurado Vargas, M., Laubenstein, M., Lee, K.B., Lee, Y.-K., Lépy, M.-C., Maringer, F.-J., Medina Peyres, V., Mille, M., Morales, M., Nour, S., Plenteda, R., Rubio Montera, M.P., Sima, O., Tomei, C., Vidmar, G., 2008. An intercomparison of Monte Carlo codes used in gamma-ray spectrometry. *Applied Radiation and Isotopes* 66, 764-768.

Vidmar, T., Capogni, M., Hult, M., Hurtado, S., Kastlander, J., Lutter, G., Lépy, M.-C., Martinkovič, J., Ramebäck, H. , Sima, O., Tzika, F., Vidmar, G., 2014. Equivalence of computer codes for calculation of coincidence summing correction factors. *Applied Radiation and Isotopes* 87, 336–341.

Figure captions:

Figure 1: Geometrical model for the case of water source with p-type detector (“AW” case).

Figure 2: Visualisation of the MCNP prepared detector geometry.

Figure 3-a: Mean value of the full-energy peak and total efficiencies (FEPE and TE) calculated for detector A for the 4 samples (The plotted lines have no meaning and are only to guide the eye).

Figure 3-b: Mean value of the full-energy peak and total efficiencies (FEPE and TE) calculated for detector B for the 4 samples (The plotted lines have no meaning and are only to help the eye).

Figure 4: Example of GEANT4 test for detector A and point source using 4 options: quadratic sum (of the 5 energies) of the relative differences (%) related to the mean value.

Figure 5: Relative difference between full-energy peak efficiencies for detector A with point and filter sources calculated by MCNP, with and without the lead shielding.

Table captions:

Table 1: Main simulation parameters used in the different codes.

Table 2: Calculated value and associated uncertainty obtained with EGSnrc (1 participant).

Table 3: Mean value and standard deviation of the GEANT4 participant’s results for the eight study cases.

Table 4: Mean value and standard deviation of the GESPECOR participant’s results for the eight study cases.

Table 5: Mean value and standard deviation of the MCNP participant’s results for the eight study cases.

Table 6: Mean value and standard deviation of the PENELOPE participant’s results for the eight study cases.

Table 7: Mean value and standard deviation of the participant’s final results for the eight study cases

Figures:

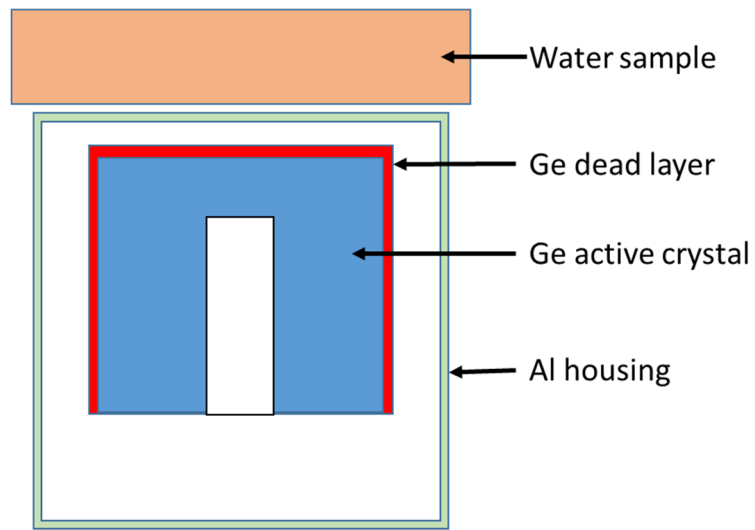


Figure 1: Geometrical model for the case of water source with p-type detector ("AW" case).

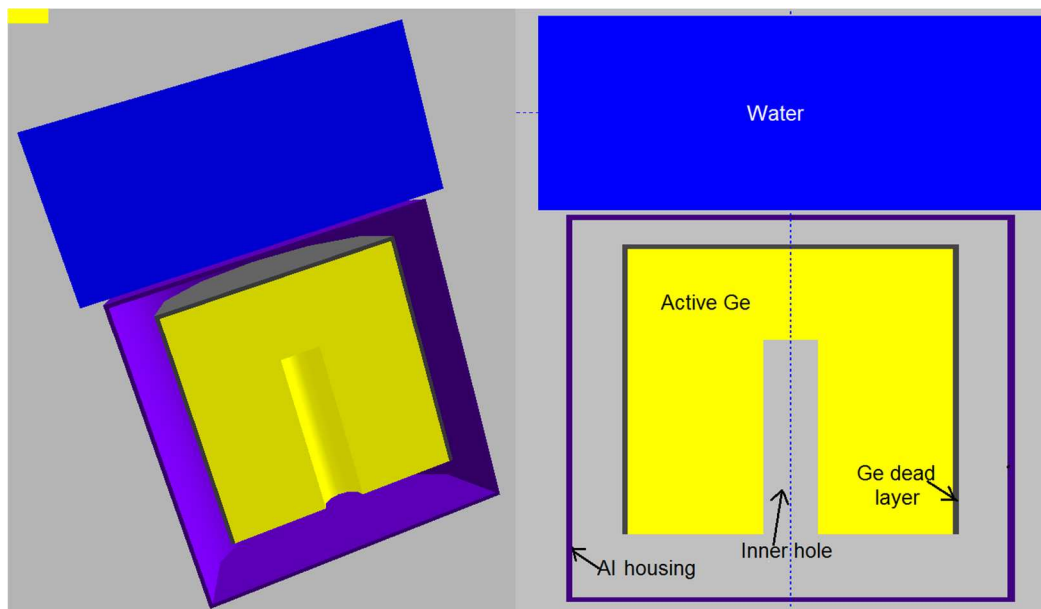


Figure 2: Visualisation of the MCNP prepared detector geometry ("AW")

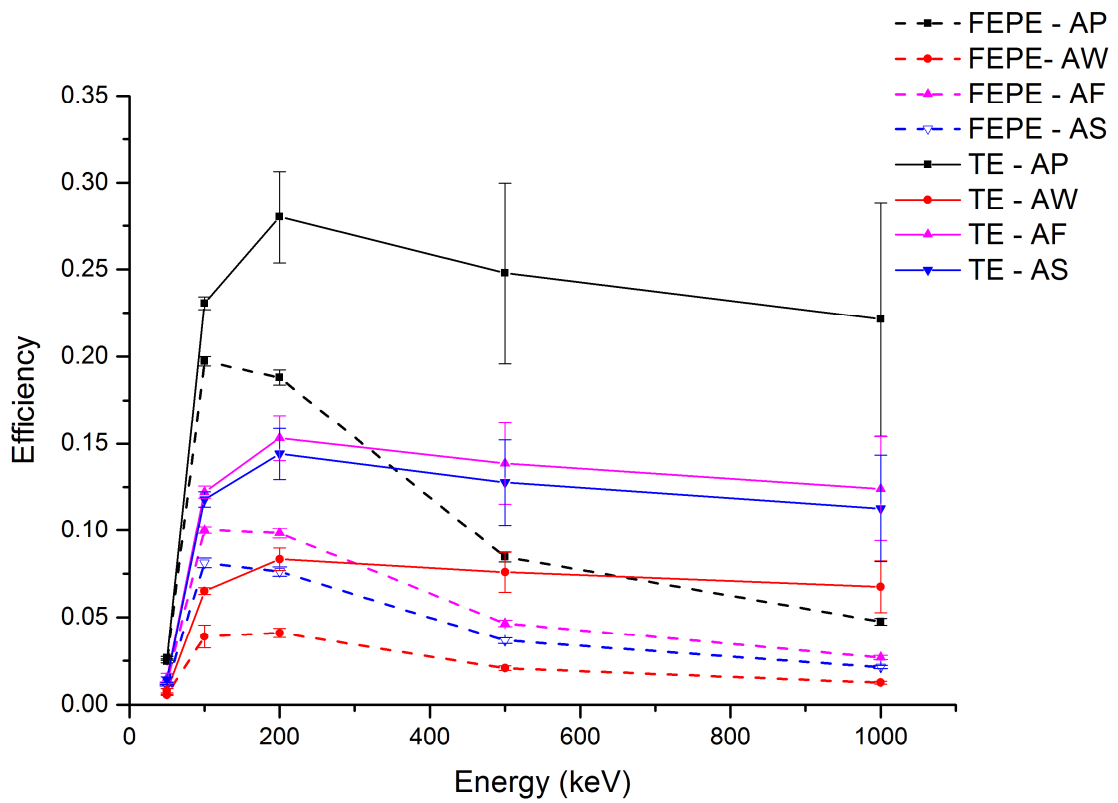


Figure 3-a: Mean value of the full-energy peak and total efficiencies (FEPE and TE) calculated for detector A for the 4 samples.
 (The plotted lines have no meaning and are only to guide the eye)

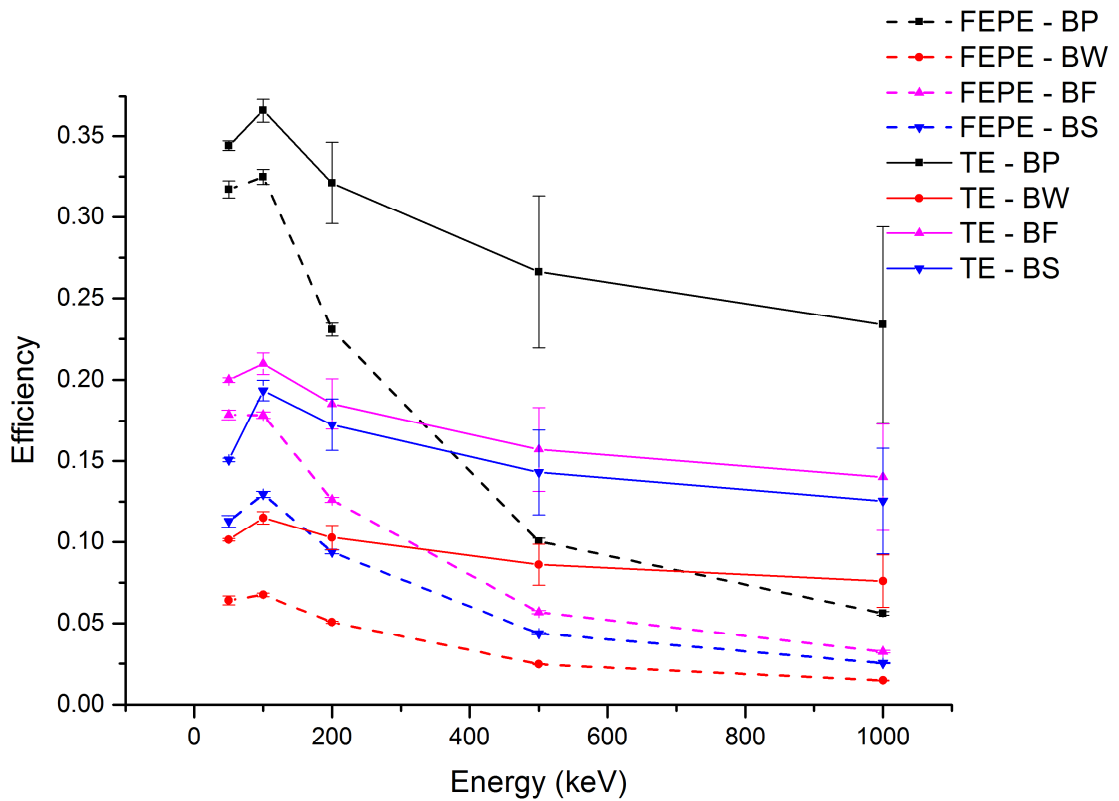


Figure 3-b: Mean value of the full-energy peak and total efficiencies (FEPE and TE) calculated for detector B for the 4 samples. (The plotted lines have no meaning and are only to help the eye)

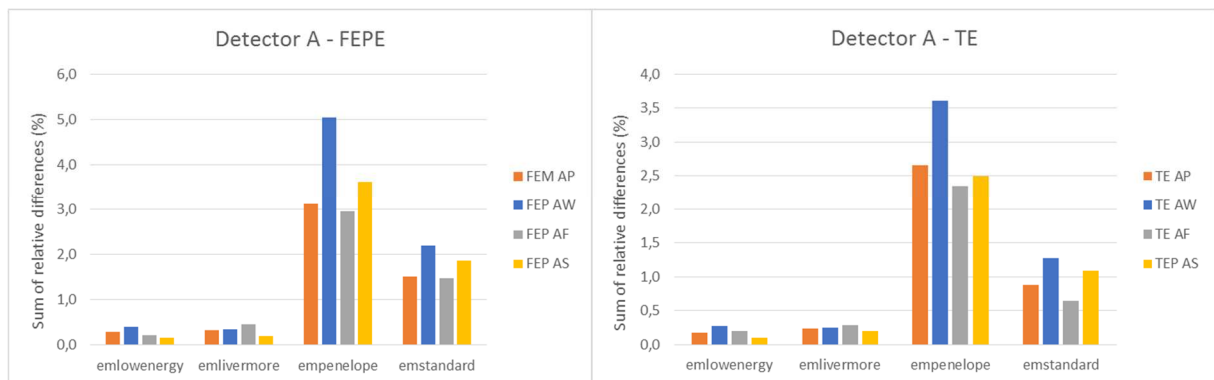


Figure 4: Example of GEANT4 test for detector A and point source using 4 options: quadratic sum (of the 5 energies) of the relative differences (%) related to the mean value.



Figure 5: Relative difference between full-energy peak efficiencies for detector A with point and filter sources calculated by MCNP, with and without the lead shielding.

Tables:

Code	Energy cuts for secondary particles :	Number of channels	Detection threshold	Peak energy sigma (if applicable)	Number of generated events	Number of users
EGSnrc	1 keV (e-, e+ and photons)	1000	Not applicable	Not applicable	1.0E7	1
GEANT4	0.25 keV (e-, e+ and photons)	Not applicable	1 keV	1.0 keV	1.0E7	4
GESPECOR Version 4.2	1.9 keV (photons) 10 keV (electrons)	Not applicable		Not applicable	1.0E6	2
MCNP	1 keV (e-, e+ and photons)	1000	1.0 keV	1.0 keV	1.0E8	4
PENELOPE	1 keV (e- and photons) 10 keV (e+)	1000	0.5 keV	Not applicable	1.0E7	6

Table 1: Main simulation parameters used in the different codes

E (keV)	AP		BP		AW		BW		AF		BF		AS		BS	
	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)	Mean Value	Relative uncertainty (%)
Full-energy peak efficiency																
50	0,0243	0,20	0,3167	0,05	0,0055	0,43	0,0627	0,12	0,0126	0,28	0,1770	0,07	0,0113	0,30	0,1145	0,09
100	0,1974	0,06	0,3263	0,05	0,0404	0,15	0,0673	0,12	0,1003	0,09	0,1779	0,07	0,0811	0,11	0,1297	0,08
200	0,1893	0,07	0,2327	0,06	0,0408	0,12	0,0509	0,14	0,0989	0,10	0,1258	0,08	0,0764	0,11	0,0940	0,10
500	0,0857	0,10	0,1015	0,09	0,0210	0,17	0,0249	0,20	0,0471	0,14	0,0568	0,13	0,0370	0,16	0,0438	0,15
1000	0,0482	0,14	0,0570	0,13	0,0127	0,21	0,0151	0,26	0,0273	0,19	0,0327	0,17	0,0218	0,21	0,0257	0,19
Total efficiency																
50	0,0269	2E-05	0,3448	5E-06	0,0076	4E-05	0,1015	1E-05	0,0143	3E-05	0,2010	6E-06	0,0141	3E-05	0,1579	8E-06
100	0,2299	6E-06	0,3673	4E-06	0,0657	1E-05	0,1168	9E-06	0,1232	9E-06	0,2123	6E-06	0,1184	9E-06	0,1958	7E-06
200	0,2722	6E-06	0,3154	5E-06	0,0830	9E-06	0,1024	1E-05	0,1521	8E-06	0,1827	7E-06	0,1413	8E-06	0,1691	7E-06
500	0,2284	7E-06	0,2513	6E-06	0,0733	9E-06	0,0826	1E-05	0,1330	9E-06	0,1493	8E-06	0,1208	9E-06	0,1348	9E-06
1000	0,1941	7E-06	0,2136	7E-06	0,0636	9E-06	0,0709	1E-05	0,1158	9E-06	0,1298	9E-06	0,1034	1E-05	0,1147	9E-06

Table 2: Calculated value and associated uncertainty obtained with EGSnrc (1 participant).

E (keV)	AP		BP		AW		BW		AF		BF		AS		BS	
	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)
Full-energy peak efficiency																
50	0.0248	1.08	0.3199	0.14	0.0060	1.43	0.0658	2.53	0.0130	1.49	0.1804	0.19	0.0115	1.12	0.1155	0.37
100	0.1982	0.17	0.3271	0.18	0.0412	0.32	0.0683	0.43	0.1012	0.35	0.1796	0.20	0.0820	0.36	0.1309	0.44
200	0.1896	0.25	0.2328	0.28	0.0411	0.57	0.0509	0.63	0.0996	0.22	0.1268	0.20	0.0771	0.17	0.0947	0.28
500	0.0854	0.45	0.1015	0.07	0.0209	0.32	0.0250	0.16	0.0472	0.19	0.0570	0.20	0.0369	0.79	0.0437	0.36
1000	0.0479	0.27	0.0565	0.28	0.0127	1.12	0.0150	0.54	0.0273	0.66	0.0327	0.69	0.0217	0.61	0.0256	0.79
Total efficiency																
50	0.0269	1.16	0.3448	0.14	0.0076	1.09	0.1014	0.13	0.0143	1.34	0.1999	0.07	0.0136	0.87	0.1504	0.17
100	0.2276	0.13	0.3628	0.13	0.0636	0.29	0.1121	0.22	0.1202	0.18	0.2061	0.18	0.1156	0.15	0.1895	0.29
200	0.2708	0.12	0.3127	0.13	0.0814	0.11	0.0993	0.11	0.1499	0.14	0.1794	0.22	0.1398	0.21	0.1660	0.22
500	0.2270	0.21	0.2502	0.12	0.0725	0.15	0.0814	0.15	0.1319	0.12	0.1480	0.12	0.1199	0.19	0.1333	0.25
1000	0.1930	0.10	0.2125	0.19	0.0629	0.14	0.0697	0.18	0.1146	0.23	0.1284	0.25	0.1024	0.17	0.1137	0.32

Table 3: Mean value and standard deviation of the GEANT4 participant's results for the eight study cases.

E (keV)	AP		BP		AW		BW		AF		BF		AS		BS	
	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)
Full-energy peak efficiency																
50	0.0238	0.02	0.3058	0.01	0.0053	0.01	0.0608	0.11	0.0120	0.10	0.1719	0.02	0.0102	0.28	0.1070	0.11
100	0.1899	0.02	0.3158	0.00	0.0378	0.08	0.0653	0.00	0.0946	0.00	0.1732	0.02	0.0747	0.02	0.1251	0.04
200	0.1765	0.00	0.2237	0.06	0.0372	0.04	0.0490	0.18	0.0909	0.11	0.1220	0.05	0.0694	0.39	0.0906	0.14
500	0.0771	0.13	0.0971	0.13	0.0184	0.22	0.0238	0.07	0.0416	0.08	0.0546	0.14	0.0324	0.31	0.0418	0.18
1000	0.0426	0.12	0.0541	0.01	0.0110	0.17	0.0143	0.35	0.0236	0.21	0.0311	0.09	0.0189	0.25	0.0244	0.27
Total efficiency																
50	0.0429	0.34	0.3394	0.17	0.0111	0.68	0.0994	0.17	0.0224	0.21	0.1966	0.17	0.0185	0.45	0.1485	0.20
100	0.2291	0.15	0.3543	0.11	0.0627	0.54	0.1098	0.00	0.1184	0.03	0.2011	0.26	0.1121	0.27	0.1865	0.09
200	0.2533	0.04	0.3032	0.13	0.0753	0.08	0.0971	0.03	0.1376	0.23	0.1742	0.01	0.1282	0.56	0.1625	0.26
500	0.2085	0.00	0.2432	0.04	0.0656	0.65	0.0793	0.45	0.1187	0.11	0.1440	0.27	0.1086	0.28	0.1311	0.34
1000	0.1765	0.01	0.2046	0.09	0.0567	0.64	0.0681	0.51	0.1026	0.39	0.1237	0.09	0.0922	0.32	0.1103	0.43

Table 4: Mean value and standard deviation of the GESPECOR participant's results for the eight study cases

E (keV)	AP		BP		AW		BW		AF		BF		AS		BS	
	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)
Full-energy peak efficiency																
50	0.0241	3.08	0.3176	1.54	0.0056	3.31	0.0641	2.66	0.0125	2.80	0.1798	0.62	0.0113	2.28	0.1126	1.85
100	0.1979	0.32	0.3244	1.91	0.0407	0.86	0.0675	0.69	0.1008	0.38	0.1793	0.26	0.0833	0.68	0.1298	0.54
200	0.1898	0.68	0.2302	2.38	0.0408	0.33	0.0508	0.13	0.0994	0.42	0.1268	0.65	0.0783	0.14	0.0942	0.14
500	0.0864	2.03	0.1003	2.66	0.0209	0.04	0.0249	0.11	0.0474	1.67	0.0574	1.73	0.0377	0.14	0.0438	0.11
1000	0.0485	3.07	0.0560	2.84	0.0127	0.23	0.0149	0.13	0.0275	2.45	0.0329	2.59	0.0221	0.13	0.0256	0.22
Total efficiency																
50	0.0256	5.80	0.3445	0.07	0.0076	0.13	0.1013	0.10	0.0135	6.10	0.1997	0.05	0.0138	0.05	0.1502	0.05
100	0.2277	1.51	0.3649	0.75	0.0646	2.05	0.1140	2.59	0.1206	2.29	0.2086	1.51	0.1189	1.01	0.1918	1.42
200	0.2719	0.02	0.3136	0.56	0.0821	1.22	0.1005	1.97	0.1508	0.33	0.1811	0.47	0.1428	0.67	0.1673	1.12
500	0.2291	0.79	0.2500	0.50	0.0727	0.71	0.0817	0.93	0.1330	0.63	0.1494	0.54	0.1222	0.42	0.1339	0.56
1000	0.1948	0.85	0.2113	1.19	0.0631	0.63	0.0702	0.76	0.1160	1.01	0.1297	0.92	0.1046	0.36	0.1140	0.42

Table 5: Mean value and standard deviation of the MCNP participant's results for the eight study cases

E (keV)	AP		BP		AW		BW		AF		BF		AS		BS	
	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)
Full-energy peak efficiency																
50	0.0244	0.87	0.3171	0.18	0.0056	0.85	0.0629	0.35	0.0127	0.40	0.1778	0.11	0.0110	0.72	0.1113	0.41
100	0.1979	0.13	0.3262	0.13	0.0406	0.30	0.0673	0.30	0.1009	0.24	0.1786	0.16	0.0810	0.19	0.1293	0.19
200	0.1887	0.36	0.2315	0.22	0.0407	0.37	0.0506	0.53	0.0991	0.05	0.1261	0.09	0.0763	0.34	0.0939	0.13
500	0.0849	0.72	0.1008	0.19	0.0208	0.56	0.0247	0.38	0.0469	0.33	0.0567	0.44	0.0367	0.21	0.0437	0.38
1000	0.0478	0.28	0.0563	0.14	0.0126	0.44	0.0149	0.65	0.0271	0.44	0.0323	0.30	0.0215	0.76	0.0254	0.44
Total efficiency																
50	0.0270	0.86	0.3451	0.21	0.0077	0.63	0.1015	0.37	0.0143	0.40	0.1999	0.06	0.0137	0.53	0.1509	0.17
100	0.2302	0.10	0.3665	0.19	0.0657	0.35	0.1164	0.32	0.1229	0.13	0.2107	0.26	0.1178	0.11	0.1941	0.17
200	0.2709	0.59	0.3138	0.46	0.0826	0.47	0.1015	0.70	0.1509	0.29	0.1813	0.48	0.1406	0.43	0.1684	0.44
500	0.2270	0.53	0.2502	0.28	0.0730	0.51	0.0822	0.30	0.1321	0.59	0.1484	0.50	0.1203	0.42	0.1343	0.36
1000	0.1939	0.28	0.2128	0.27	0.0633	0.19	0.0706	0.25	0.1151	0.12	0.1288	0.17	0.1031	0.14	0.1142	0.12

Table 6: Mean value and standard deviation of the PENELOPE participant's results for the eight study cases

E (keV)	AP		BP		AW		BW		AF		BF		AS		BS	
	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)	Mean Value	Relative standard deviation (%)
Full-energy peak efficiency																
50	0.0244	2.10	0.3180	0.91	0.0057	3.01	0.0640	2.50	0.0127	2.10	0.1791	0.71	0.0112	2.06	0.1128	1.76
100	0.1980	0.21	0.3258	1.08	0.0408	0.76	0.0676	0.73	0.1009	0.32	0.1791	0.28	0.0820	1.29	0.1298	0.51
200	0.1893	0.52	0.2314	1.36	0.0408	0.44	0.0507	0.49	0.0993	0.31	0.1265	0.46	0.0772	1.18	0.0942	0.36
500	0.0856	1.32	0.1008	1.49	0.0208	0.43	0.0248	0.52	0.0471	1.02	0.0570	1.13	0.0370	1.31	0.0437	0.33
1000	0.0481	1.80	0.0562	1.57	0.0126	0.64	0.0149	0.54	0.0273	1.49	0.0326	1.66	0.0218	1.29	0.0255	0.50
Total efficiency																
50	0.0267	2.71	0.3449	0.17	0.0076	1.00	0.1015	0.28	0.0142	2.90	0.1998	0.07	0.0136	0.80	0.1506	0.24
100	0.2289	0.75	0.3650	0.55	0.0648	1.69	0.1145	1.96	0.1216	1.29	0.2088	1.14	0.1172	1.14	0.1922	1.20
200	0.2711	0.43	0.3134	0.40	0.0821	0.83	0.1006	1.31	0.1506	0.40	0.1806	0.64	0.1407	0.84	0.1674	0.82
500	0.2276	0.44	0.2502	0.25	0.0728	0.50	0.0818	0.56	0.1322	0.54	0.1485	0.50	0.1205	0.74	0.1339	0.48
1000	0.1938	0.45	0.2125	0.49	0.0632	0.40	0.0702	0.62	0.1151	0.55	0.1288	0.48	0.1031	0.75	0.1140	0.29

Table 7: Mean value and standard deviation of the participant's final results for the eight study cases