PENELOPE

Some information about how it works

Preparation of the input files for the action

INFORMATION

- We are presently working with PENELOPE 2016
- Two main programs
  - PENCYL (Cylindrical geometries)
  - PENMAIN (Any type of geometry)
- FORTRAN modules - Require compilation to get the executable files

More information about the physical interactions taken into account : *Overview of physical interaction models for photon and electron transport used in Monte Carlo codes,* Francesc Salvat and José M Fernández-Varea, Metrologia **46** (2009) S112–S138

PURPOSE

PENELOPE simulates coupled electron-photon transport in arbitrary material systems

consisting of a number of homogeneous regions (bodies) limited by sharp (and passive)

interfaces.

Initially, it was devised to simulate the PENetration and Energy LOss of Positrons and Electrons in matter; photons were introduced later.

PREPARATION OF THE INFORMATION

- Define a geometry:
  - Shapes
  - Material

- Input the parameters of the different materials
- Create a «*.in » file containing these information

MATERIALS

PENELOPE reads the required physical information about each material (which includes tables of physical properties, interaction cross sections, relaxation data, etc.) from an input material data file.

The material data file is created by means of the auxiliary program material

MATERIAL.EXE

- Used to create one database for one material

  - Either we use the predefined materials using the reference number
  - Or input the chemical characteristics of the material

- *** ELEMENTS (id. number = atomic number):
- 1 Hydrogen 34 Selenium 67 Holmium
- 2 Helium 35 Bromine 68 Erbium
- 3 Lithium 36 Krypton 69 Thulium
- 4 Beryllium 37 Rubidium 70 Ytterbium
- 5 Boron 38 Strontium 71 Lutetium
- 6 Amorphous carbon 39 Yttrium 72 Hafnium
- 7 Nitrogen 40 Zirconium 73 Tantalum
- 8 Oxygen 41 Niobium 74 Tungsten
- 9 Fluorine 42 Molybdenum 75 Rhenium
- 10 Neon 43 Technetium 76 Osmium
- 11 Sodium 44 Ruthenium 77 Iridium
- 12 Magnesium 45 Rhodium 78 Platinum
- 13 Aluminum 46 Palladium 79 Gold
- 14 Silicon 47 Silver 80 Mercury
- 15 Phosphorus 48 Cadmium 81 Thallium
- 16 Sulfur 49 Indium 82 Lead
- 17 Chlorine 50 Tin 83 Bismuth
- 18 Argon 51 Antimony 84 Polonium
- 19 Potassium 52 Tellurium 85 Astatine
- 20 Calcium 53 Iodine 86 Radon
- 21 Scandium 54 Xenon 87 Francium
- 22 Titanium 55 Cesium 88 Radium
- 23 Vanadium 56 Barium 89 Actinium
- 24 Chromium 57 Lanthanum 90 Thorium
- 25 Manganese 58 Cerium 91 Protactinium
- 26 Iron 59 Praseodymium 92 Uranium
- 27 Cobalt 60 Neodymium 93 Neptunium
- 28 Nickel 61 Promethium 94 Plutonium
- 29 Copper 62 Samarium 95 Americium
- 30 Zinc 63 Europium 96 Curium
- 31 Gallium 64 Gadolinium 97 Berkelium
- 32 Germanium 65 Terbium 98 Californium
- 33 Arsenic 66 Dysprosium 99 Einsteinium

*** COMPOUNDS AND MIXTURES (in alphabetical order):

100 Acetone
101 Acetylene
102 Adenine
103 Adipose tissue (ICRP)
104 Air, dry (near sea level)
105 Alanine
106 Aluminum oxide
107 Amber
108 Ammonia
109 Aniline
110 Anthracene
111 B-100 bone-equivalent plastic
112 Bakelite
113 Barium fluoride
114 Barium sulfate
115 Benzene
116 Beryllium oxide
117 Bismuth germanium oxide
118 Blood (ICRP)
119 Bone, compact (ICRU)
120 Bone, cortical (ICRP)
121 Boron carbide
122 Boron oxide
123 Brain (ICRP)
124 Butane
125 N-butyl alcohol
126 C-552 air-equivalent plastic
127 Cadmium telluride
128 Cadmium tungstate
129 Calcium carbonate
130 Calcium fluoride
131 Calcium oxide
132 Calcium sulfate
133 Calcium tungstate

Up to 280

Cylindrical geometry

- PENCYL executable file will be used
- The geometry characteristics are included in the input file
  - Consider successive layers by increasing Z
    - Defined by Zmin and Z max and number of the layer
    - Eventually position of the center (by default, 0,0,0)
  - For each layer, consider one or several cylinders
  - Cylinders are defined by their material (number corresponding to the *.mat file), internal and external
- A « body » is the combination of a certain cylinder in a certain layer

All dimensions in cm

Energy spectrum

- In the input file : specific command to get the information on deposited energy in a specific body (crystal active layer)
- >>>>>>> Energy-deposition detectors (up to 25).
- ENDETC 0.0 500.e3 180 [Energy window and number of bins]
- EDSPC spc-enddet-01.dat [Output spectrum file name, 20 chars]

Raw results:

```
#  Results from PENMAIN. Output from energy-deposition detector #  1
#  Deposited energy spectrum.
#  WARNING: May be strongly biased if interaction forcing is used!
#  1st column: deposited energy (eV).
#  2nd column: probability density (1/(eV*particle)).
#  3rd column: statistical uncertainty (3 sigma).
 1.047500E+03  1.139501E-09  1.21E-09
 1.142500E+03  1.566815E-09  1.42E-09
 1.237500E+03  1.851690E-09  1.54E-09
 1.332500E+03  1.424377E-09  1.35E-09
 1.427500E+03  8.546261E-10  1.05E-09
 1.522500E+03  9.970638E-10  1.13E-09
 1.617500E+03  1.139501E-09  1.21E-09
 1.712500E+03  8.546261E-10  1.05E-09
 1.807500E+03  8.546261E-10  1.05E-09
 1.902500E+03  1.281939E-09  1.28E-09
 1.997500E+03  1.281939E-09  1.28E-09
 2.092500E+03  1.139501E-09  1.21E-09
```

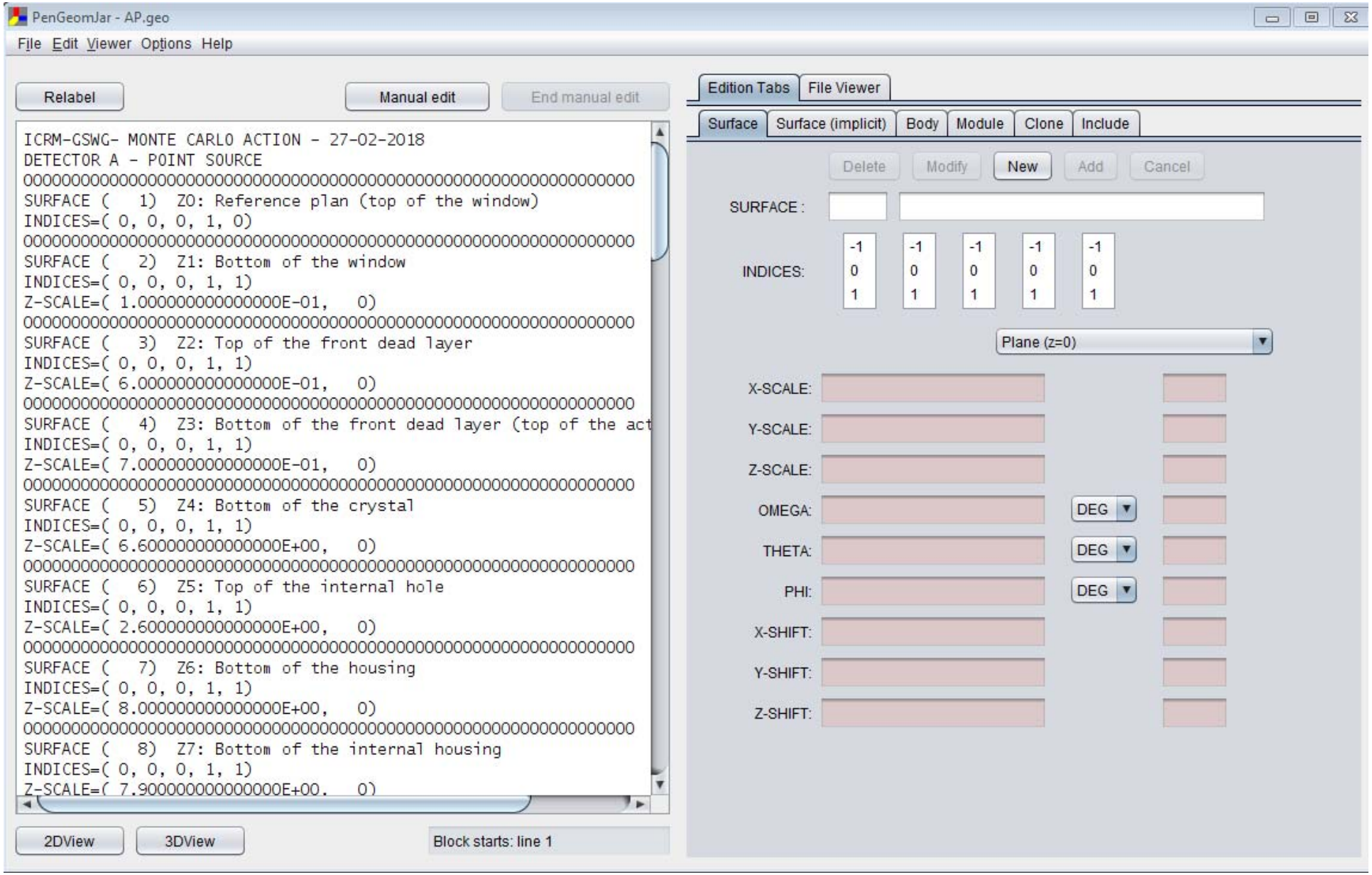
Penmain

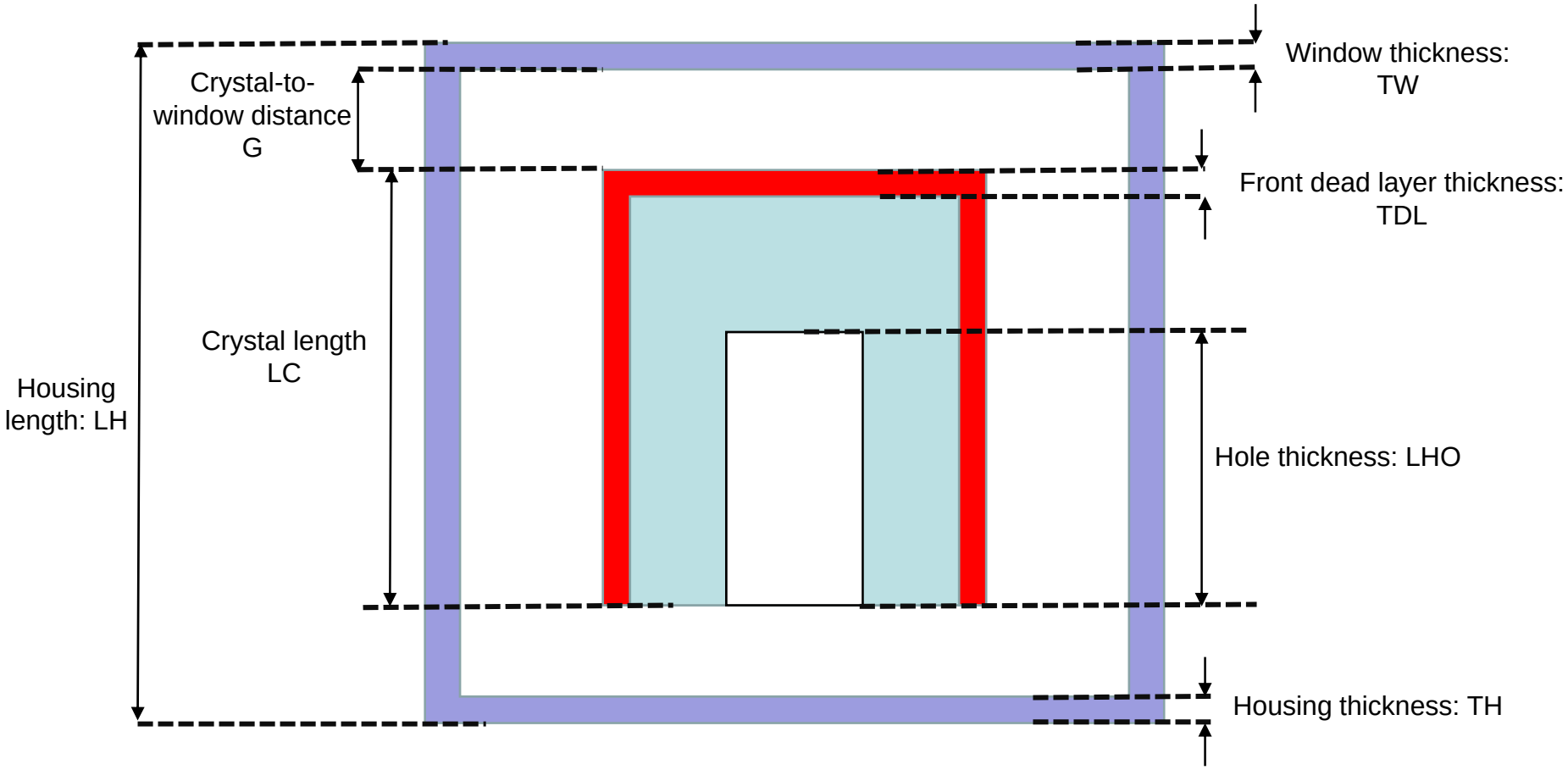
- For more complicated geometries
  - Need to prepare an external geometry file
  - Prepare a material file (including all necessary materials)
  - Prepare an input file

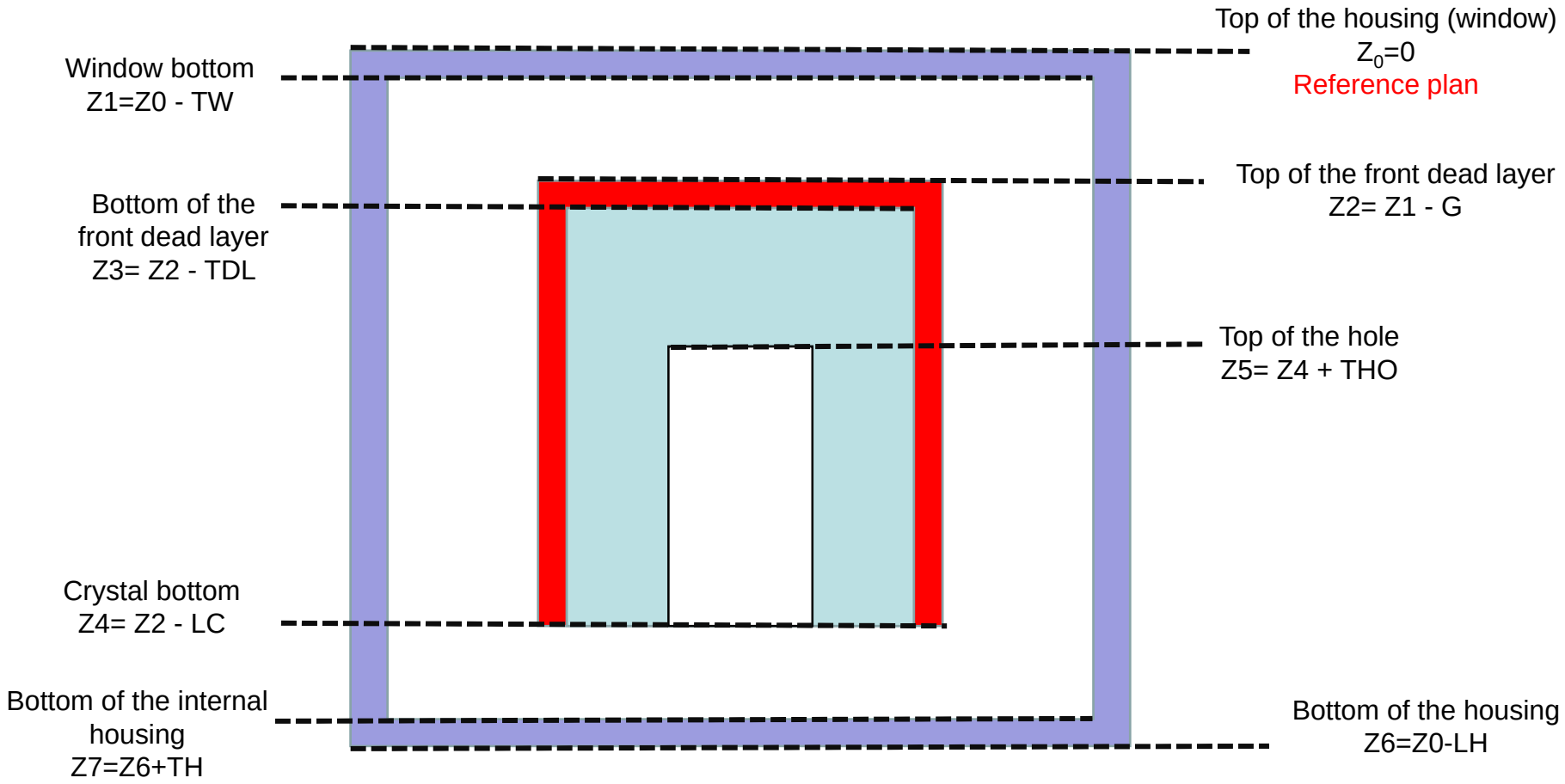
Preparing geometry

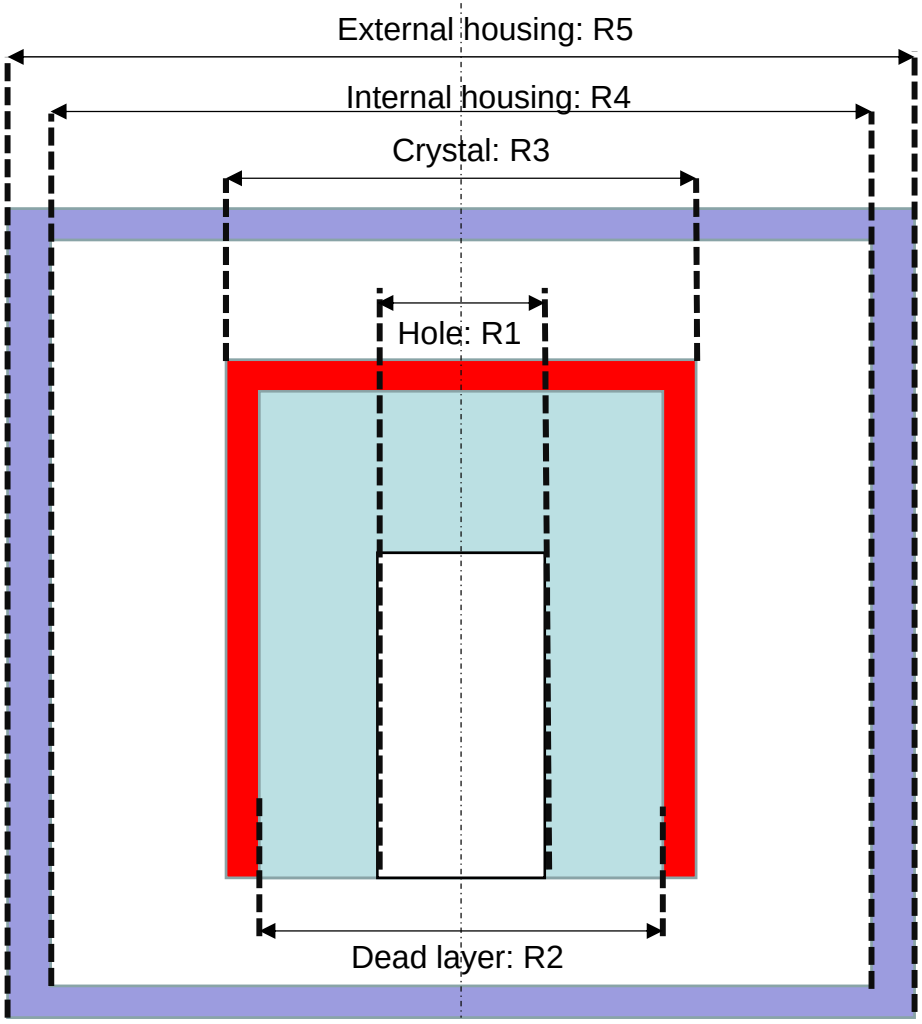
- Define limiting surface
  - Surfaces are defined by parameters of a quadric equation
  - Envetuyally shift and rotation
- Define bodies
  - Constituting material (number corresponding to the mat file)
  - Limiting surfaces (in or out)

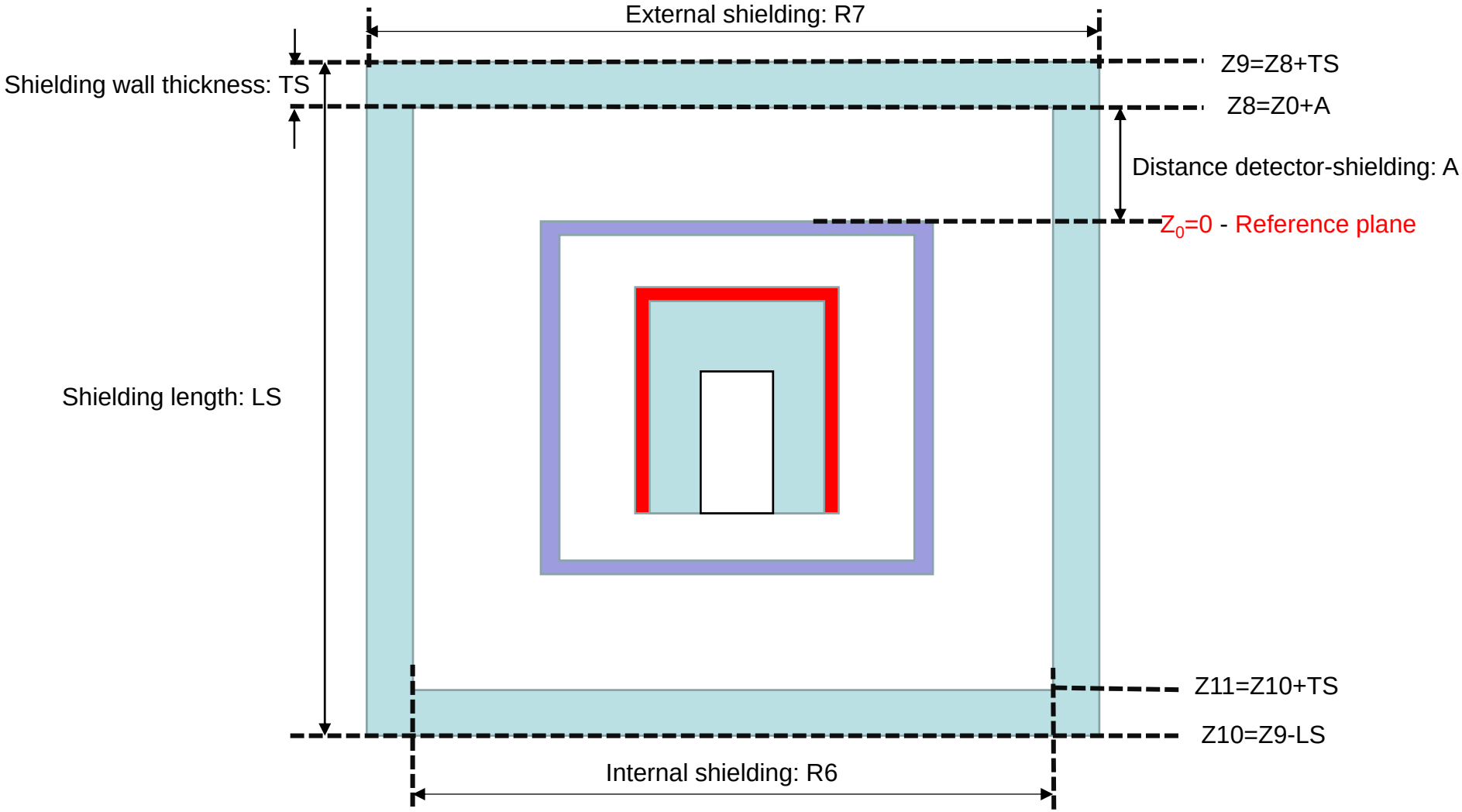
Preparing and checking the geometry: Pengeomjar

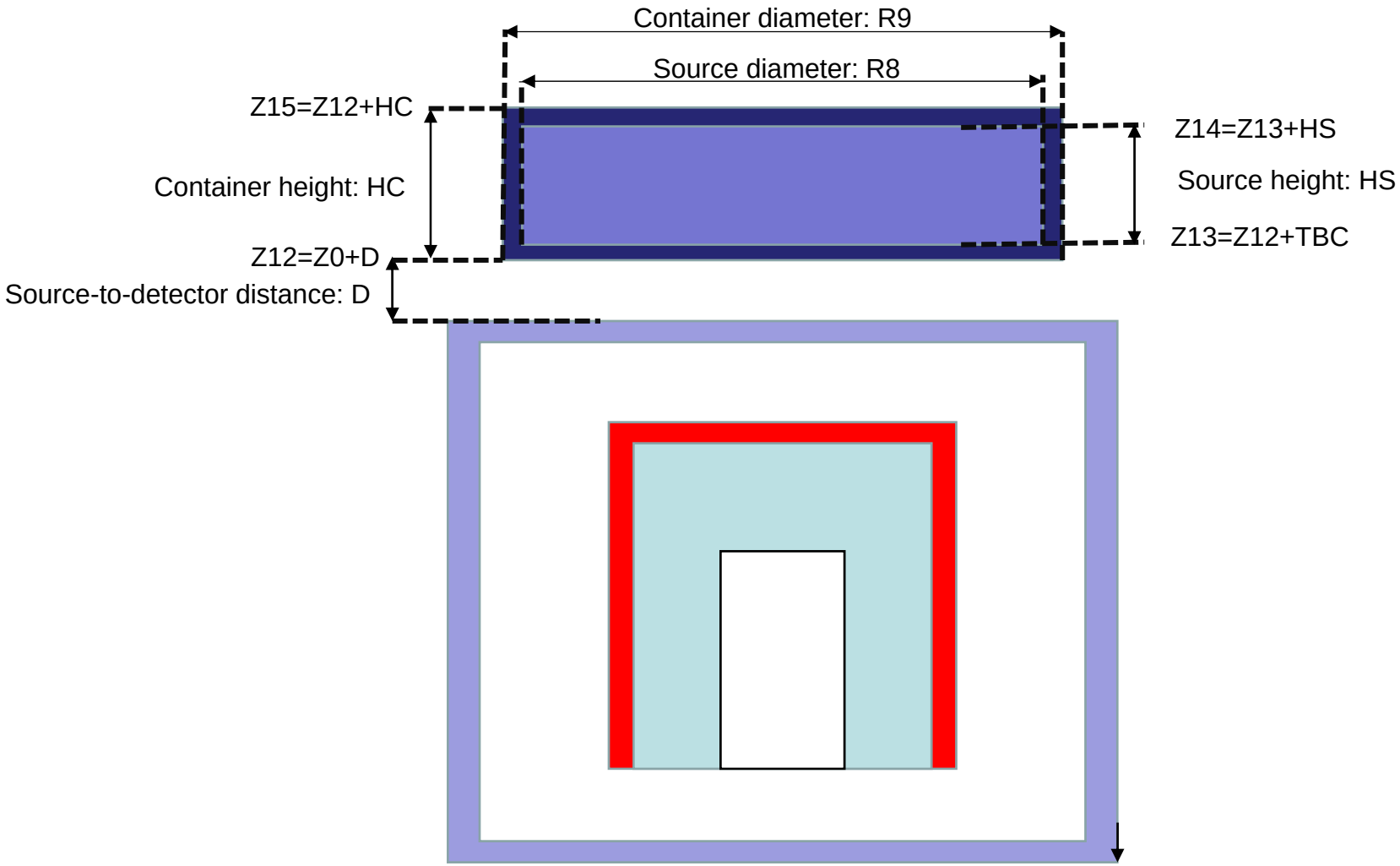



Window thickness:
TW
Crystal-to-
window distance
G
Front dead layer thickness:
TDL
Crystal length
LC
Housing
length: LH
Hole thickness: LHO
Housing thickness: TH


Top of the housing (window)
Z_0=0
Reference plan
Window bottom
Z1=Z0 - TW
Top of the front dead layer
Z2= Z1 - G
Bottom of the
front dead layer
Z3= Z2 - TDL
Top of the hole
Z5= Z4 + THO
Crystal bottom
Z4= Z2 - LC
Bottom of the internal
housing
Z7=Z6+TH
Bottom of the housing
Z6=Z0-LH


External housing: R5
Internal housing: R4
Crystal: R3
Hole: R1
Dead layer: R2


External shielding: R7
Shielding wall thickness: TS
Z9=Z8+TS
Z8=Z0+A
Distance detector-shielding: A
Z_0=0 - Reference plane
Shielding length: LS
Z11=Z10+TS
Z10=Z9-LS
Internal shielding: R6


Container diameter: R9
Source diameter: R8
Z15=Z12+HC
Container height: HC
Z12=Z0+D
Source-to-detector distance: D
Z14=Z13+HS
Source height: HS
Z13=Z12+TBC

GEOMETRY PARAMETERS

				Detector A	Detector B	
Parameter	**Detector A**	**Detector B**		**Dimension (cm)**	**Dimension (cm)**	
Crystal material	Ge	Ge				
Crystal diameter (including the side dead slayer)	60	60	=2*R3	6	6	
Crystal length (including the top dead layer)	60	60	LC	6	6	
Dead layer thickness (top and side)	1	0	TDL	0.1	0	
Hole diameter	10	10	=2*R1	1	1	
Hole depth	40	40	LHO	4	4	
Window diameter	80	80	=2*R5	8	8	
Window thickness	1	1	TW	0.1	0.1	
Window material	Al	Al				
Crystal-to-window distance	5	5	G	0.5	0.5	
Housing length	80	80	LH	8	8	
Housing thickness	1	1	TH	0.1	0.1	
Housing material	Al	Al				
Shielding diameter	400	400	=2*R7	40	40	
Shielding length	400	400	LS	40	40	
Shielding thickness	50	50	TS	5	5	
Gap between detector housing and external shielding	110	110	A	11	11	
Shielding material	Pb	Pb				
Cylindrical sources				Source Water	Source Soil	Source Filter
Container diameter			=2*R9	9	6	8
Container height			HC	4	2	0.3
Container side thickness			TSC	0	0	0
Container bottom thickness			TBC	0	0	0
Container material	vacuum	vacuum				
Source diameter			=2*R8	9	6	8
Source height			HS	4	2	0.3
Source-to-detector distance	1	1	D	0.1	0.1	0.1

GEOMETRY PARAMETERS

			Detector A	Detector B						
		Position (de	Position (cm)							Surfaces
Detector	Z0	0	0	0						1
	Z1	Z0-TW	-0.1	-0.1						2
	Z2	Z1-G	-0.6	-0.6						3
	Z3	Z2-TDL	-0.7	-0.6						4
	Z4	Z2-LC	-6.6	-6.6						5
	Z5	Z4+LHO	-2.6	-2.6						6
	Z6	Z0-LH	-8	-8						7
	Z7	Z6+TH	-7.9	-7.9						8
Shielding										
	Z8	Z0+A	11	11						9
	Z9	Z8+TS	16	16						10
	Z10	Z9-LS	-24	-24						11
	Z11	Z10+TS	-19	-19						12
Source			Water		Soil		Filter			
	Z12	Z0+D	0.1	0.1	0.1	0.1	0.1	0.1		13
	Z13	Z12+TBC	0.1	0.1	0.1	0.1	0.1	0.1		14
	Z14	Z12+HC	4.1	4.1	2.1	2.1	0.4	0.4		15
	Z15	Z13+HS	4.1	4.1	2.1	2.1	0.4	0.4		16
Detector	R1	R1	0.5	0.5						17
	R3	R3	3	3						18
	R2	R3-TDL	2.9	3						19
	R5	R5	4	4						20
	R4	R5-TH	3.9	3.9						21
Shielding	R7	R7	20	20						22
	R6	R7-TS	15	15						23
			Water		Soil		Filter			
Source	R8	R8	4.5	4.5	3	3	4	4		24
	R9	R9	4.5	4.5	3	3	4	4		25

Example of input file

```
TITLE  DETECTOR A WITH POINT SOURCE
    .
    >>>>>>>> Source definition.
SKPAR  2       [Primary particles: 1=electron, 2=photon, 3=positron]
SENERG 1.0E6                    [Initial energy, in eV]
SPOSIT 0 0 0.1                  [Source position: X0,Y0,Z0 in cm]
SCONE  0 0 180                  [Beam direction: THETA,PHI in deg]
    .
    >>>>>>>> Material data and simulation parameters.
MFNAME Ge.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Al.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Water.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Polyeth.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Air.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Pb.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
    .
    >>>>>>>> Geometry definition file.
GEOMFN AP.geo               [Geometry file name, 18 characters]
    .
    >>>>>>>> Energy deposition detectors (up to 25).
ENDETC 5e3 1.01E6 1000      [Energy window and number of channels]
EDBODY 2                    [Active body; one line for each body]
    .
    >>>>>>>> Job properties.
NSIMSH 1000000          [Desired number of showers, max=2**31-1]
TIME   50000                [Allotted simulation time, in sec]
RSEED  12345 54321              [Random number generator seeds]
```

Volume source

This can be taken into account in the input file by defining a « box » containing the source (one or several bodies)

Input file :

SKPAR KPARP [Primary particles: 1=electron, 2=photon, 3=positron]
SENERG SE0 [Initial energy (monoenergetic sources only)]
SPECTR Ei,Pi [E bin: lower-end and total probability]
SPOSIT SX0,SY0,SZ0 [Coordinates of the source]
SBOX SSX,SSY,SSZ [Source box dimensions]
SBODY KB [Active source body; one line for each body]
SCONE THETA,PHI,ALPHA [Conical beam; angles in deg]
SPYRAM THETAL,THETAU,PHIL,PHIU [Rectangular beam; angles in deg]

Main results

Point source – B Detector

E (keV)	Moyenne	Ecart-type	E-type relatif (%)
50	0.3171	0.0006	0.18
100	0.3262	0.0004	0.13
200	0.2315	0.0005	0.22
500	0.1008	0.0002	0.19
1000	0.0562	0.0001	0.21

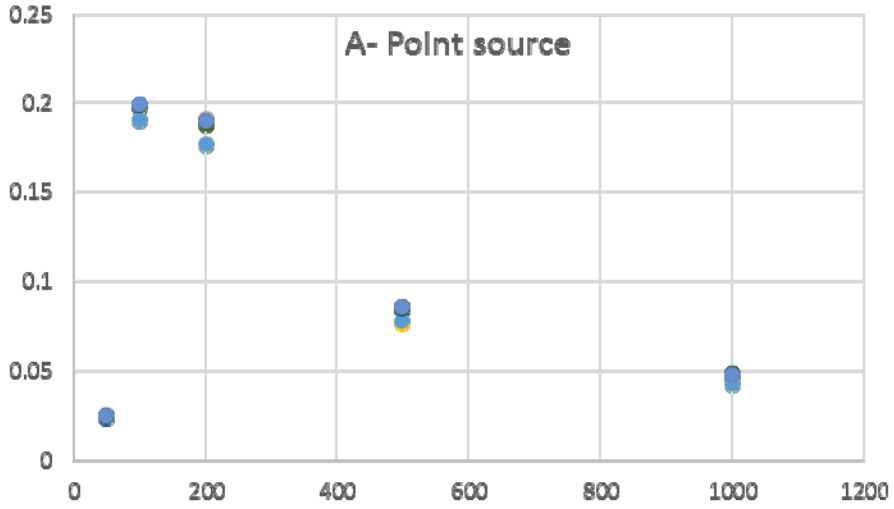
Soil source – A Detector

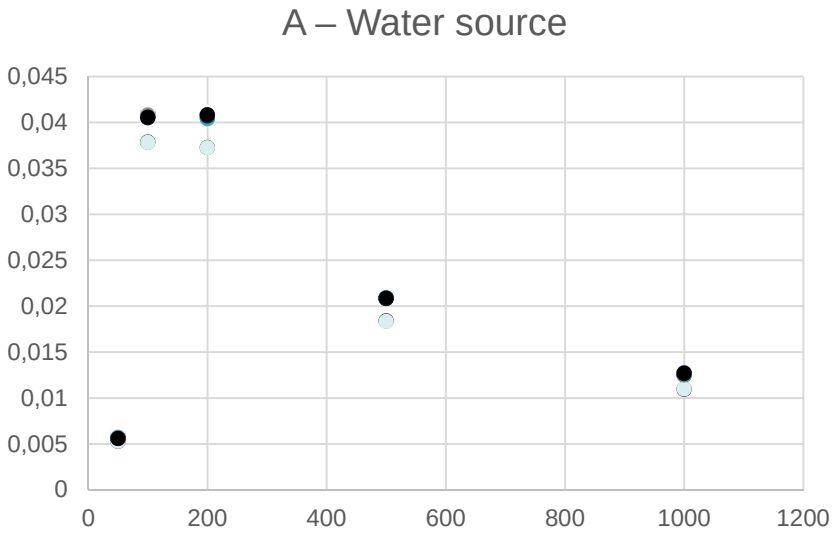
E (keV)	Moyenne	Ecart-type	E-type relatif (%)
50	0.0111	0.0003	2.57
100	0.0818	0.0018	2.15
200	0.0769	0.0014	1.82
500	0.0369	0.0006	1.58
1000	0.0217	0.0004	1.81

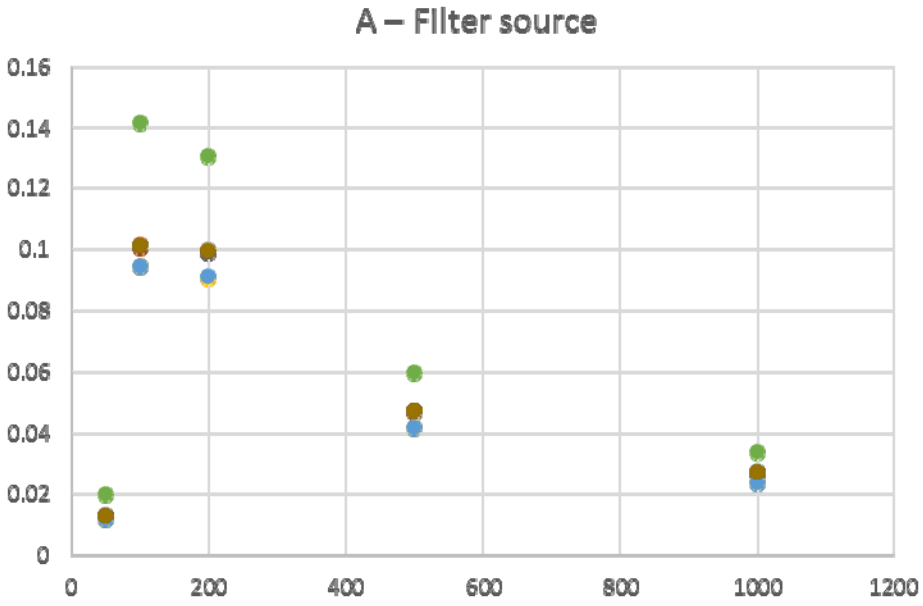
- 3 versions (2011, 2014 and 2016)

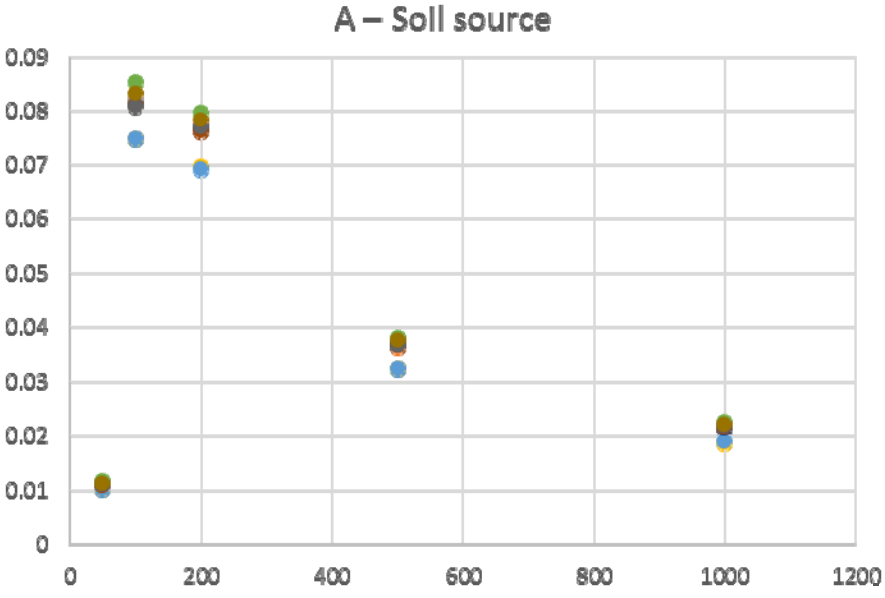
Haoran	Ming	NTUA	Marilia	Marie-Christin	antinos PENE
2.46E-02	2.46E-02	2.44E-02	2.45E-02	2.40E-02	2.46E-02
1.98E-01	1.98E-01	1.98E-01	1.98E-01	1.98E-01	1.98E-01
1.89E-01	1.89E-01	1.89E-01	1.89E-01	1.88E-01	1.88E-01
8.54E-02	8.53E-02	8.56E-02	8.49E-02	8.39E-02	8.47E-02
4.75E-02	4.77E-02	4.80E-02	4.77E-02	4.80E-02	4.78E-02
2014	2016	2011			

Detector A

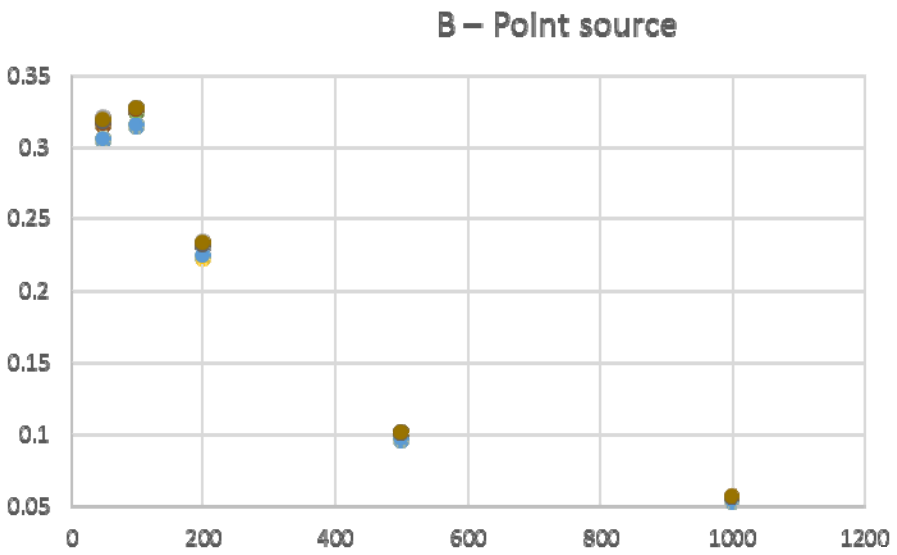

A- Point source
0.25
0.2
0.15
0.1
0.05
0
0
200
400
600
800
1000
1200

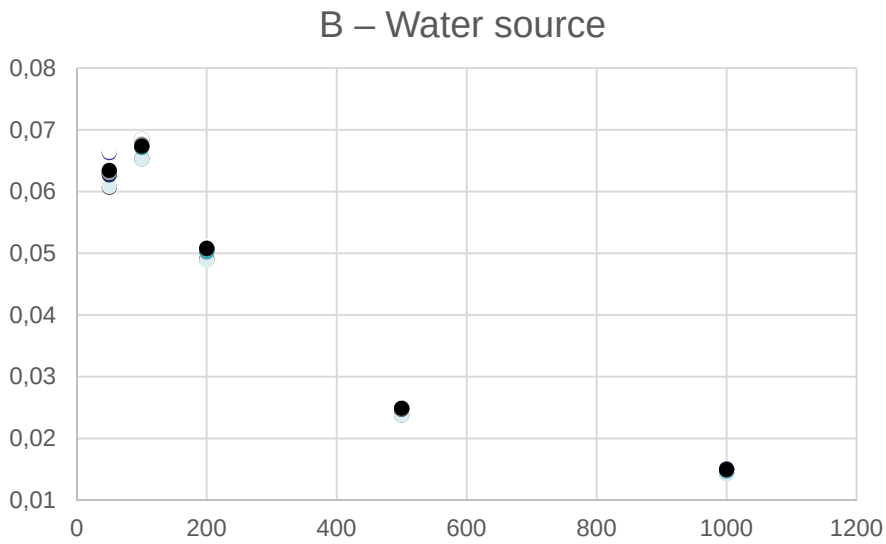

A – Water source
0,045
0,04
0,035
0,03
0,025
0,02
0,015
0,01
0,005
0
0
200
400
600
800
1000
1200

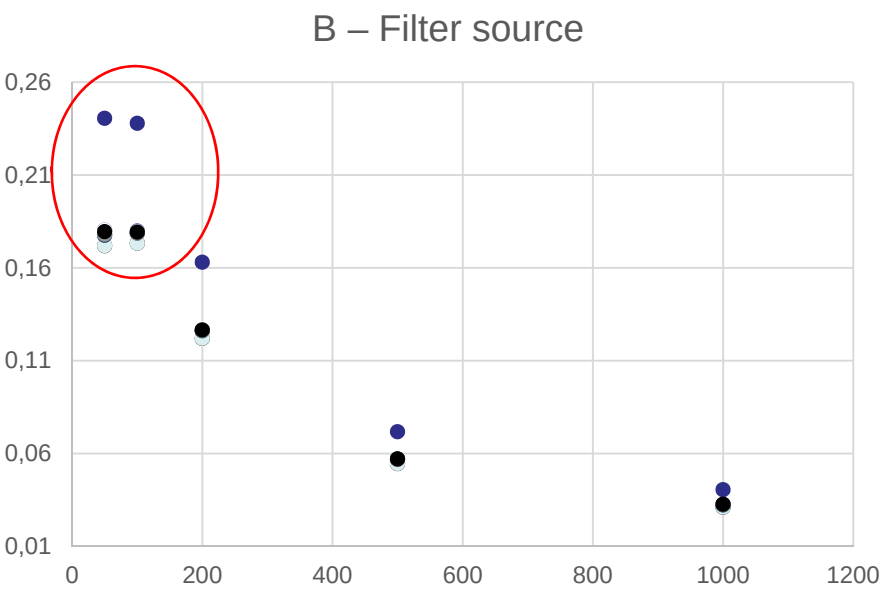

A – Filter source
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0
200
400
600
800
1000
1200

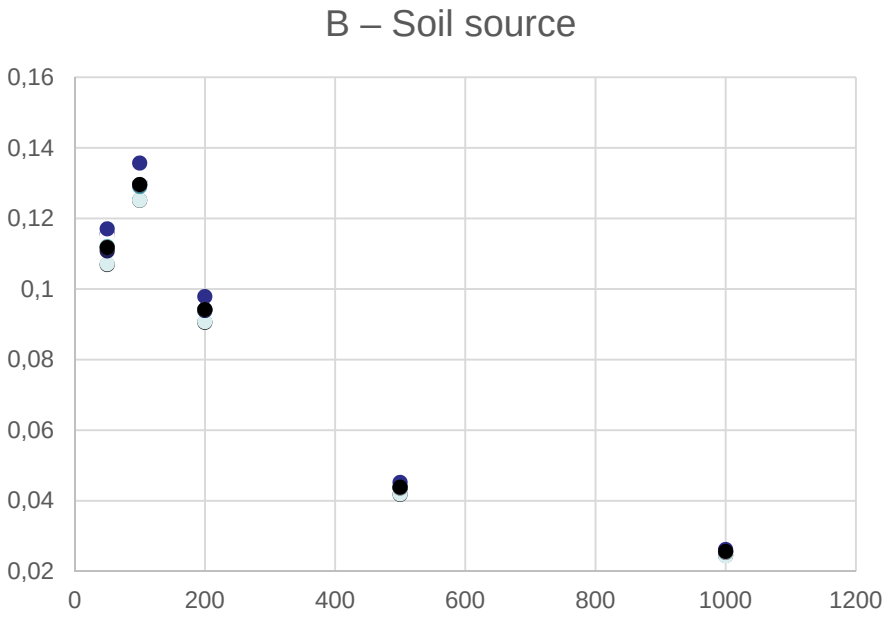

A – Soil source
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
200
400
600
800
1000
1200

Detector B


B – Point source
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
200
400
600
800
1000
1200


B – Water source
0,08
0,07
0,06
0,05
0,04
0,03
0,02
0,01
0
200
400
600
800
1000
1200


B – Filter source
0,26
0,21
0,16
0,11
0,06
0,01
0
200
400
600
800
1000
1200


B – Soil source
0,16
0,14
0,12
0,1
0,08
0,06
0,04
0,02
0
200
400
600
800
1000
1200

Synthesis

		Point		Water		Filter		Soil	
	E (keV)	Mean	Standard deviation (%)	Mean	Standard deviation (%)	Mean	Standard deviation (%)	Mean	Standard deviation (%)
A Detector	50	0.0244	1.51	0.0056	4.05	0.0132	15.71	0.0110	3.97
	100	0.1968	1.56	0.0403	2.76	0.1032	11.48	0.0809	3.70
	200	0.1871	2.54	0.0402	3.29	0.1003	9.48	0.0760	4.09
	500	0.0840	3.67	0.0205	4.57	0.0472	9.11	0.0363	4.94
	1000	0.0470	4.23	0.0124	5.10	0.0271	8.81	0.0213	5.30
B Detector	50	0.0244	1.51	0.0634	2.95	0.1825	9.67	0.1121	2.71
	100	0.1968	1.56	0.0672	1.46	0.1826	9.16	0.1295	2.01
	200	0.1871	2.54	0.0504	1.39	0.1285	8.17	0.0939	1.91
	500	0.0840	3.67	0.0246	1.64	0.0576	7.50	0.0436	1.98
	1000	0.0470	4.23	0.0148	1.61	0.0328	7.13	0.0254	1.89

Checking of results on-going.