

MONTCARL

MONTE-CARLO

SIMULATION

MONTCARL

M O N T E - C A R L O S I M U L A T I O N
O F L I G H T S C A T T E R I N G A N D A B S O R P T I O N ,
F L U O R E S C E N C E A N D R A M A N - S C A T T E R I N G
I N T U R B I D M E D I A

Frits F.M. de Mul - www.demul.net/frits - June 2016

This program may be used freely, provided proper reference is made when you want to publish results obtained with it, to:

- F.F.M. de Mul, M.H. Koelink, M.L. Kok, P.J. Harmsma, J. Greve, R. Graaff, J.G. Aarnoudse, "Laser Doppler Velocimetry and Monte Carlo Simulations on Models for Blood Perfusion in Tissue", Applied Optics, vol. 34, 1995, p. 6595-6611.
- De Mul, F.F.M.; Monte-Carlo simulation of Light transport in Turbid Media, Chapter 12 in: Handbook of Coherent Domain Optical Methods, Biomedical Diagnostics, Environment and Material Science, Tuchin, Valery V. (Ed.), 2004, XLII, 1004 p. (2-volume-set), Kluwer Publishers, Hardcover ISBN: 1-4020-7576-6, pages 465-533.
- De Mul, F.F.M.; Monte-Carlo simulation of Light transport in Turbid Media, Chapter 15 in: Handbook of Coherent Domain Optical Methods, Biomedical Diagnostics, Environment and Material Science, Tuchin, Valery V. (Ed.), 2013, Springer Publishers, Hardcover ISBN: 978-1-4614-5176-1, pages 593-661.
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==== 0. GENERAL OBJECTIVE OF THE PROGRAM ====

The program calculates Monte-Carlo simulations of LIGHT SCATTERING and/or ABSORPTION (optional: followed by FLUORESCENCE or RAMAN-scattering, or PHOTOACOUSTICS) in turbid media, like tissue.

The SAMPLE may consist of a single or more LAYERS, each with its own absorption and scattering data, in the form of concentrations of scattering particles embedded in a medium.

In order to register DOPPLER spectra, to each type of scattering particle a certain velocity vector can be given.

In each layer a number of separately defined structures (called "OBJECTS") with rectangular, cylindrical, spherical, torusses or conical shape) may be present, with similar characteristics as the layers.

With those objects e.g. blood vessels can be mimicked.

Also an oblique mirror plane can be inserted.

Furthermore, the layers may be subdivided into sublayers (depth pixels, see below).

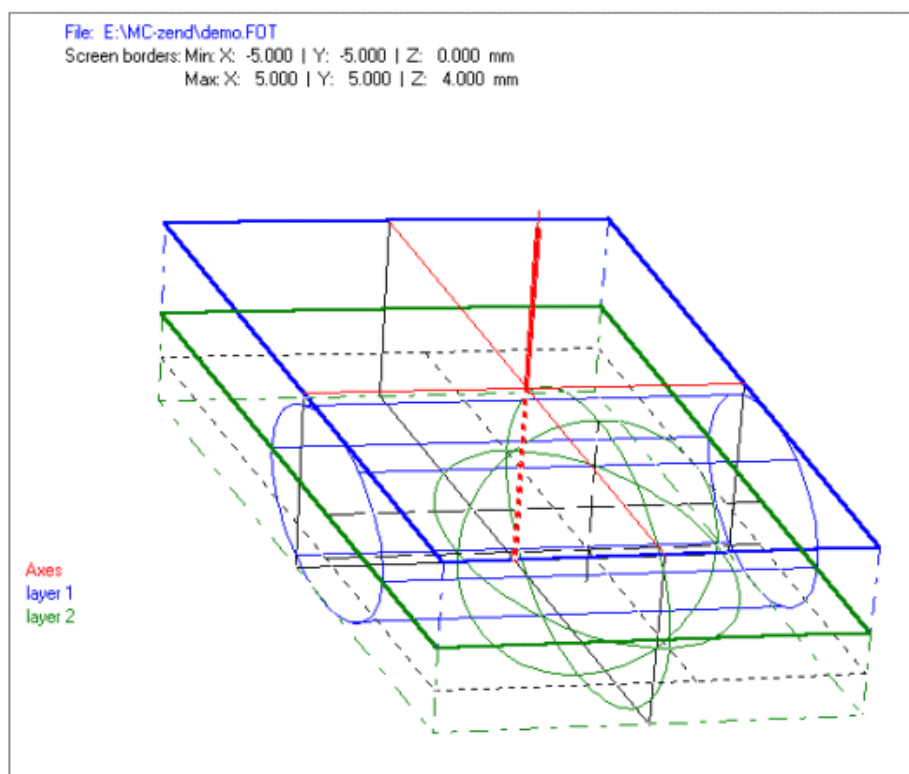


Fig. 1. Structure plot of a two-layer system with a horizontal cylindrical tube and asphere (see section 2), filled with various concentrations of scattering/absorbing particles. Laser light (here diverging beam) injected around Z-axis.

NB. All plots in this document were produced using the MONTCARL-program output facilities.

-> MORE FIGURES AT THE END OF THIS REPORT.

There are a number of options: internal light sources and external beams, internal and external detection, plots of distributions of various variables (photon positions, path length distributions, photon tracking, layer+object structure plots, frequency modulation by Fourier transformations, angular distributions, photoacoustic response plots,.etc. etc.

==== 1. PHOTON TRANSPORT : LAYERS AND OBJECTS ====

The program calculates Monte-Carlo simulations of LIGHT SCATTERING and/or ABSORPTION (optional: followed by FLUORESCENCE or RAMAN-scattering, or PHOTOACOUSTICS) in turbid media, like tissue.

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In order to register DOPPLER spectra, to each type of scattering particle a certain velocity vector can be given.

In each layer a number of separately defined structures (called "OBJECTS"): with rectangular, cylindrical, spherical or conical shape) may be present, with similar characteristics as the layers.

With those objects e.g. blood vessels can be mimicked.

Also an oblique mirror plane can be inserted.
Furthermore, the layers may be subdivided into sublayers (depth pixels, see below).

==== 2. MONTCARL - README.1ST - file ====

The Montcarl package contains following files:

- MC20xx.EXE : executable file (Windows-version), (program version 20.xx)
- README.1st : this introduction
- MONTCARL.TXT : this ASCII-text file with HELP information.
- DEMO.INP : This file is a demo-input file with some structures in the scattering medium.
- DEMO.MIE : A file with the scattering function for DEMO.INP

==== 3. INPUT AND OUTPUT OF PHOTON DATA ====

= INPUT FILES:

- *.INP FILE, *.LST AND *.MIE-FILE(S): data with settings for simulations.
For details: see below.
- *.RSP : for type-R objects: coordinates of random spheres.

= OUTPUT FILES: The program has the following file output:

- *.FOx : (x=0..9,T) containing the photon data, as described below;
 - *.INF : Ascii-file containing general data about the simulation, such as:
 - + total number of photons reflected, absorbed, transmitted;
 - + average numbers;
 - + data of the scatterers, layers and objects;
 - *.2D : 2-dim. plots of the variables of ALL detected photons;
 - *.3Da : 3-dim. plots of the <scatter depth> or absorption depth of ALL detected photons.
 - *.3Dd : id. of Doppler photons.
 - *.PAT : file of tracking path xyz-positions (optional) (in units as with storage in *.FOT-file, see below), each path preceded by a dummy position: x,y,z = 9999,9999,# of following positions)
 - *.DIK : used by the program: internal values.
 - *.MCn : (n=1,2..) temporary files with settings;
- In case a simulation run is interrupted during execution:
- .IRP : data (in internal format) to resume the simulation.

In case calculation of photo-acoustic response is available:

- *.ABS : 3-dim. voxels with # of absorbed photons.
- *.PAI : settings to calculate photo-acoustic time response
- *.PAC : photo-acoustic time-response results at array of detectors.
- *.PAG : id. for grouped array detector.

For the formats used, see below.

BEFORE RUNNING THE PROGRAM:

1. Create directories (= folders) for:

- *.MIE-files: Scattering functions (and copy DEMO.MIE in it);
- *.INP-files: Input-files (ASCII), and *.LST-files (Ascii: series list);
- *.FOT-files (and other output files): Storage of detected photons.

2. Copy *.INP- and *.MIE-files in the respective directories.

3. Start the program, read DEMO.INP and change its data lines containing the MIE- and FOT-directory names, using the EDIT-INP option, or with a text processor.

==== 4. PHOTOACOUSTICS AND FLUORESCENCE/RAMAN ====

The program is also capable of calculating the FLUORESCENCE/RAMAN or PHOTOACOUSTIC response of photons absorbed inside the structure, to be detected at an array of detectors at the surface.

The calculation consists of several steps:

1. Calculate of a FOT-file with positions of photons, absorbed at the wavelength of absorption; and a PAT-file with tracking path positions (optional);
2. (FLUORESCENCE/RAMAN): Using this file as photon source, calculate scattering at the wavelength of emission with a fresh INP-file. To handle a fluorescence/Raman SPECTRUM, a series of new INP-files can be created and simulated, with varying laser wavelengths.
3. (PHOTOACOUSTICS): Using this file as source of acoustic sources, calculate photo-acoustic response (can be done directly after calculation of absorption FOT-file). For details: see option: "Photoacoustics: details"

==== 5. PHOTON INJECTION, TRANSPORT AND DETECTION ====

There are 3 options for entering photons:

1. from the outside world, using a beam;
2. from a single point in the inside of the layer system;
3. using absorbed photons from a previously made *.FOT-file.

Ad 1. A (laser) beam impinges onto the first layer (interface 0th-1st layer).

Ad 2. The direction and divergence of the photon distribution emerging from the source point is entered.

Ad 3. This is especially useful for calculating fluorescence or Raman. The photons start from their point of absorption, in isotropic direction.

FRESNEL RELATIONS are used for describing interface crossings.

Natural polarization has been assumed throughout.

The photon is followed when traveling through the sample.

Four modes are available: detection of SCATTERING by REFLECTION and/or TRANSMISSION, or INTERNALLY, or of ABSORPTION, optionally followed by FLUORESCENCE/RAMAN-scattering.

==== 6. DETECTION OF EMERGING PHOTONS ====

The program offers various ways of detecting emerging photons:

- R: REFLECTION: upon refractive passage of the interface between two layers N-1 and N (with N=1...nr.-of-layers; N=0:surface), if directed towards negative Z-values (theta > 90 degr.)
- S: REFLECTION: the same, but different storage.
- T: TRANSMISSION: upon refractive passage of the backside of the layer system, if directed towards positive Z-values (theta < 90 degr.)
- I,J,K: INTERNAL: upon refractive passage of the surface of a sphere or the curved surface of a cylinder tube or cone, travelling from inside to outside.
- A: ABSORPTION: upon absorption in a particle or a layer or an object
- E: ALL: (= reflection + transmission + absorption)

In all cases the X and Y-position at the point of detection are stored.

In cases I,J,K and A, the real Z-position at that point is stored, but with R, S and T, the averaged scatter depth or the maximum depth is stored. Case E is a mixture.

FLUORESCENCE/RAMAN: Detection of emerging photons as above.

==== 7. COORDINATE AXES, STORAGE UNITS AND ACCURACY ====

Z-AXIS perpendicular to the surface of the sample,
pos. inward ($Z > 0$ with increasing depth in the sample)
X and Y-axes: in plane of sample surface.

STORAGE UNITS:

- = FOT-files created with `progr.version < 2018`:
 - 1 micron (default); or 10 micron (in following cases:
 - (1) for X- and Y-coords: if detection field (see below) extends beyond +/- 32768 micron (= max. for "integers")
 - (2) for Z-coords: if total thickness of layer system extends beyond 65535 micron (= max. for "words").
- = FOT-files created with `prog.version >=2018`: no limitations.

When injected from above ($Z < 0$) the photon starts at a depth of 0.1 μm underneath surface. The photon beam can be injected from within the sample as well (use the "focus"-option).

UNITS for angles: 1 degree, for Doppler frequency: 1 Hz.

==== 8. PROGRAM INTERRUPT, STOP AND BREAK ====

INTERRUPT: The execution of simulations (single or series) can be interrupted by pressing the Interrupt-button.
The relevant data are stored in a file, named after the actual *.INP-file, or - in case of a series of simulations - after the first file in the series, and will have extension *.IRP.
Afterwards the program will detect the presence of those interruption files and will ask the user about resumption.
This *.IRP-file is also created or updated at each output-to-file instant, (i.e. after each 1000 photons) enabling resumption after a program crash.

STOP: Pressing the Stop-button will stop the program but no IRP-file will be created.

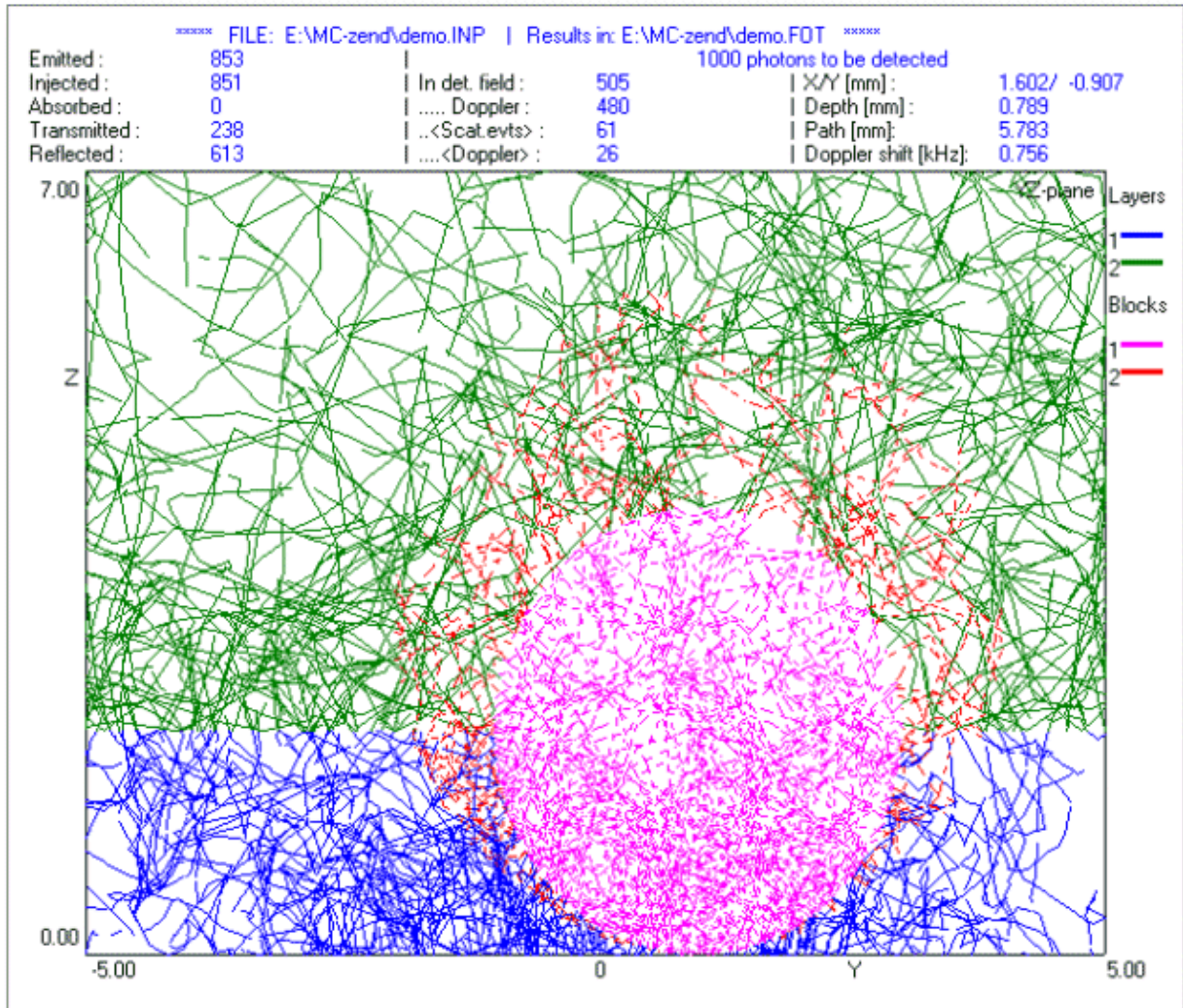


Fig. 2. Running graphics of the simulation process of the structure of fig.1. View in YZ-plane. Photons entering around pos (0,0,0). The tube (X-direction) and sphere can be seen.

==== 9. PHOTON SOURCE : wavelength, direction, dimensions, divergence ====

The program can handle :

- distributed sources (a FOT-file with absorbed photons)
- pencil beams (set divergences = 0);
- diverging beams;
- parallel beams;
- ring-shaped beams.

Each BEAM SHAPE: 2 options: Uniform/Gaussian; half-width HWHM to be entered.

If PENCIL beams and DIVERGING beams, the beam is assumed to be created in one point, called FOCUS. This focus point may be positioned within the layer system ($Z > 0$) or in front of it ($Z < 0$).

If PARALLEL BEAM, the convention is adopted that the Focus point always is situated at -1000 mm, i.e. in front of the layer system. When this value is inserted, the program assumes a lens at the surface, with a focal length of 1000 mm. In doing so a parallel beam will enter

the layer system. Here the divergence angles are used to determine the width of the beam at the surface.
If RING-shaped beam, the Tilt angles theta and phi have a different meaning (see below).

BEAM TILT: The mean direction of the beam can be tilted in 2 directions: with respect to the Z-axis (details: see below) and within the XY-plane;

(1) TILT ANGLE OF LASER BEAM with respect to Z-axis (THETA-angle):

* Angle of beam direction vector with +Z-axis (+inward) (0..180), or:

* Isotropic injection: two options: enter -1 or -2:

-1: according to: $Distribution(t)=const.$ (t=theta)

then $Cumul.funct.(t)=Integral[const.sin(t).dt]$ over 0..pi/2;

-2: according to: flux from isotropic radiance,

then $Cumul.funct.(t)=Integral[const.cos(t).sin(t).dt]$ over 0..pi/2.

then direction will be randomized at point of injection.

(2) TILT ANGLE in XY-plane with respect to X-axis (PHI-angle):

if z-focus > 0 (within layer system) and source-in-focus: add 1000 to phi.

To enter beam spot size <>0: use (focus.z=-1000) & (divergence angles<>0)!

If RING-shaped beam:

Enter: MAX.ring radius + 1000 [mm] in stead of theta,

and MIN.ring radius [mm] in stead of phi. (Rectang. distr. only!)

DIAPHRAGM: can be used to limit the beam area at the surface (optional)

if wide open: enter 1000.

==== 10. OBJECTS : Rectangular, cylindrical, spherical, conical, mirror ====

The program can handle 11 types of "OBJECTS"

(in previous versions called "Blocks"):

- RECTANGLES: The sides of these objects are parallel to the main coordinate axes (type B);
- CYLINDERS: 3 types: in X, Y, or Z-direction; (types X, Y and Z);
- SPHERES (type S), single or arranged in layers;
- RANDOM SPHERES (type R),
- OBLIQUE (type Q) ,
- CONICAL (type C),
- LENSES (type L), thick or thin,
- MIRROR PLANE (type M)
- (half) TORUS (type T).

Type-X and Y objects consist basically of a CYLINDER of INFINITE length, parallel to the X or Y axis respectively.

The basic cylinder can be multiplied in the local Z=const plane,

by entering a repetition distance. This distance is in the

Y- or X-direction for the X- or Y-type respectively.

Type-Z objects consist basically of a CYLINDER of FINITE length,

parallel to the Z axis. The minimum and maximum number of the layers in

which the Z-object extends can be entered. This basic cylinder can be multiplied in both X- and Y-direction, by entering a Repetition Distance.

Type-Q object is an OBLIQUE Z-object; no multiplication possible.

Type-S objects (SPHERES) can be multiplied in the same way as Z-objects.

Type-R objects (RANDOM SPHERES) are sub-objects,

situated in a cylindrical object (extending over 1 or more layers).

Position and radius are random; overlap allowed/excluded is optional.

Type-C objects (CONES) (in pos/neg X,Y or Z-dir.) are always single.

Type-M objects (MIRROR planes) are "thin" planes, with reflection determined by the refractive index. The direction of the normal vector is defined with directional theta and phi-angles.

Type L-objects (LENSES), thick or thin, transparent or turbid, with symmetry axis // Z-axis,

Type-T objects (half-TORUS) are half-torusses in XZ-plane, with symmetry axis // Y-axis, and the symmetry point on a layer boundary. From that boundary, the half-torus stretches out with the U-shape opening towards pos. or neg. Z-values (towards +Z-axis or -Z-axis respectively).

NB. The symmetry point (axis point) of a half-torus MUST be on a layer boundary!

CONVENTION FOR INTERSECTING OBJECTS: inside overlapping regions:

An object with lower number will penetrate in an object with higher number, and replace all properties of that object (and the layer where it is in).

Example:

If object 1 is situated within object 2, then the overlapping region will possess the properties of object 1.

If object 2 is situated within object 1, then the overlapping region will possess the properties of object 1, with the effect that in that region object 2 seems not to exist, from the photon point of view.

==== 11. CALCULATION: SINGLE OR SERIES simulations (*.LST) ====

The program is made to handle a "single" simulation (conversationally), or automatically a number of subsequent simulations (called a SERIES). If a "SERIES" of simulations is wanted, a list of *.INP-files has to be created, in the form of a *.LST-file (a text file, with the same name as that of the first file in the list). This creation can be done within the program, or using a word processor. When "SINGLE", photon paths can be followed graphically.

==== 12. OVERVIEW OF FILES : input and output ====

NB. "*" stands for the file name (e.g. ABC00123.xxx ; xxx=extension)

= **INPUT FILES: *.INP FILE, *.LST AND *.MIE-FILE(S):** see below.

= **OUTPUT FILES:** The program has the following file output:

- *.FOx : (x=0..9,T) containing the photon data, as described below;
- *.INF : Ascii-file containing general data about the simulation, such as:
 - + total number of photons reflected, absorbed, transmitted;
 - + average numbers;
 - + data of the scatterers, layers and objects;
- *.2D : 2-dim. plots of the variables of ALL detected photons;
- *.3Da : 3-dim. plots of the <scatter depth> or absorption depth of ALL detected photons.
- *.3Dd : id. of Doppler photons.
- *.PAT : file of tracking path xyz-positions (optional) (in units as with storage in *.FOT-file, see below), each path preceded by a dummy position: x,y,z = 9999,9999,# of following positions)
- *.DIK : used by the program: internal values.
- *.MCn : (n=1,2..) temporary files with settings;

In case calculation of photo-acoustic response is available:

- *.ABS : 3-dim. voxels with # of absorbed photons.

- *.PAI : settings to calculate photo-acoustic time response
- *.PAC : photo-acoustic time-response results at array of detectors.
- *.PAG : id. for grouped array detector.

==== 13. INPUT-FILES: *.MIE and *.INP: introduction ====

The program needs two (sets of) input-files:

1. A (set of) *.MIE-files (one for each type of scattering particle) (see below)
2. A *.INP-file: containing data about:
 - the laser beam;
 - the type of scattering particles and their scattering functions; (called: MIE-tables ; see below: MIE-files)
 - the layers and objects structure;
 - the detection window and the numerical aperture of the detector;
 - the type of calculation: reflection/transmission/absorption/all;
 - the nr. of photons to be injected or detected;
 - the depth pixel structure;
 - the directory for file output (*.FOT-files etc)
3. For R-type objects (random spheres):
 - *.RSP : coordinates of random spheres.

A series of INP-files can be listed in a *.LST-file, which enables to perform a SERIES OF SIMULATIONS automatically.

==== 13a .INPUT FILE: *.MIE : Scattering or Phase Functions ====

The extension *.MIE is used as a general designation for scattering functions, calculated using the Mie-formalism or otherwise. These files have to be calculated before starting a simulation. This can be done using the proper option at the start of the program.

There are several formalisms available:

- 1) dipolar, -2) Rayleigh/Gans, -3) Mie,
- 4) isotropic, -5) peaked forward (Gaussian profile),
- 6) Henyey-Greenstein, -7) Gegenbauer, -8) \cos^2 .

Options 1)..3) calculate absolute values for the scattering function (including SCATTERING CROSS SECTION values [μm^2]).

Options 4)..8) calculate phase functions only. These functions are normalised and then artificially multiplied with the total scattering cross section obtained from a Mie-calculation.

To arrive at the proper SCATTERING COEFFICIENTS [mm^{-1}] of those types of particles in the various layers and objects, in the *.INP-file the CONCENTRATIONS [mm^{-3}] of these particles must be entered.

Multiplication of the concentration with the scattering cross section results in the scattering coefficient [mm^{-1}] and the corresponding mean free path [mm] in the layer or object. These values are used to calculate the actual flight paths of the photons.

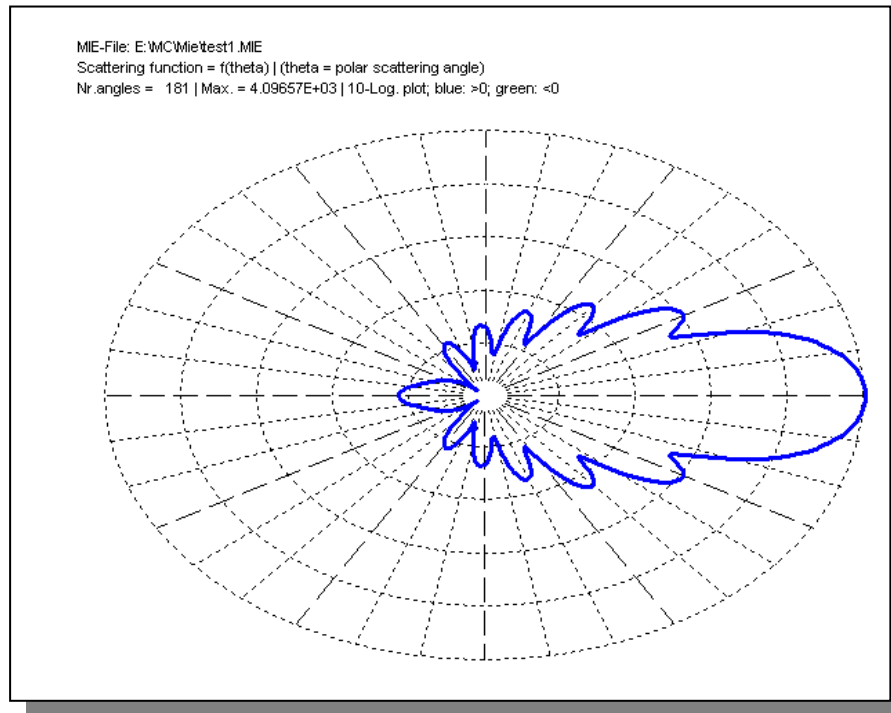


Fig. 3. Example of a MIE-file. Scattering function according to the Mie-formalism.

CONTENTS OF MIE-FILES: (file of extended: 10 bytes reals)

- nr. of angles, starting with theta=0 (zero), max. 181 values!
 - for each angle:
 - + angle (rads),
 - + resulting scattering function value at this angle,
 - + cumulative function value,
 (the cumul.function is normalised to 1 (one) at highest angle value)
 - cumul.function at max. angle (before normalisation) * overall factor =
 - = (aspect ratio)² * Q_{scatt.} / 2 ,
 - with Q_{scatt.} = scattering cross section / geometrical cross section,
 - relative refractive index of scattering particles with respect to medium,
 - aspect ratio of the particles,
 - for each contributing scattering function:
 - sequence nr. and contributing factor (and g, if Henyey-Greenstein);
 - wavelength in medium (optional)
- Sequence nrs. of contributing functions in the program:
- | | |
|-------------------------------------|------------------------------|
| 0. Overall multiplication factor | 5. Henyey-Greenstein |
| 1. Entered by keyboard or otherwise | 6. Isotropic |
| 2. Dipolar | 7. Gegenbauer |
| 3. Rayleigh-Gans | 8. Peaked forward (Gaussian) |
| 4. Mie | 9. Cos ² |

==== 13b. INPUT FILE: *.INP : input data about sample and scattering ====

For each simulation an Ascii-text file with input data is needed. These files are called *.INP files. They may be created within the program itself, using the appropriate option in the start menu, or may be created using a word processor, in Ascii-type output files. From one *.INP-file a SET of other *.INP files, in which several variables are altered subsequently, can be constructed.

For this purpose another option in the main menu is present.
 This option is useful when planning a SERIES of subsequent simulations
 (*.INP-file names in the series can be listed in *.LST).

```

    20                U                1.300
** Photon source data    1.100                0.000E+00
**                    0.000E+00                -1.000
    780.0            2.000                1.000
    10.000           ** Layer 2 **                3.000
    10.000           1.000E-01                3.000
    0.000            0.000                0.000
    0.00            1.500                1
   -10.00           0.000E+00                ** Calcul & Detect **
   100.000          5.000                S
    1.0000          ** Object 1 **                -5.000
    1.0000          X                5.000
** Nr.                1.000E-01                -5.000
scatts/layers/objects  0.000                5.000
**                    1.300                1.000
    1                0.000E+00                ** Depth pixels **
    2                1.000                5
    2                1.000                25
E:\MC-zend           2.000                ** File output **
** Scatterer 1 **    2.000                E:\MC-zend
demo                 0.000                B
0.000E+00            1                L
** Layer 1 **        ** Object 2 **        ** Nr of photons **
1.000E-01            S                D1000
    1.000            1.000E-01
X                    0.000

```

Fig.4. Example of an *.INP-file (file DEMO.INP, producing the structure of Fig.1.)

CONTENTS OF THE *.INP FILES

- NB.=> **Lines starting with "***"** : Comment lines,
 will be skipped while reading.
 These lines may be inserted freely by the user.
- => Lines starting with ">"** : data to be entered in *.INP-file
 => All entries on separate lines (unless indicated otherwise)!!!!
- > ** PHOTON SOURCE (e.g. laser beam) **
 - > WAVELENGTH [nm]
 - > If photons to be produced from internal absorption (for fluoresc./Raman):
 Enter: Name (incl dir.+ ext.) of FOT-file containing absorbed photons.
 ==> JUMP to: input of "REFRACTIVE INDEX of medium in front of
 the system of layers" !!!
 - > If photons produced from 1 single source point (e.g. laser beam or 1 point
 inside the layer system): enter:
 Beam DIVERGENCE angle (HWHM) : X-direction [degr.]
 - > Beam DIVERGENCE angle (HWHM) : Y-direction [degr.]
 (Gaussian/Rectangular distribution: enter angles x +1/-1)
 - PARALLEL (//) beam:
 enter Depth of focus = -1000 mm
 (At focus=-1000 mm & HWHM=1 mm ==> angle = 0.001 rad = 0.057296 degr.)
 (to make // beam: program assumes a positive lens at the surface)

RING-shaped beam: see below: "theta" and "phi".

- > THETA: tilting angle of beam vector with +Z-axis: (0..180) [degr.]
or: for Isotropic injection: enter -1, -2 or -3 (see at: LASER BEAM).
- > PHI: angle of beam vector in XY-plane with +X-axis: (0..360) [degr.]
(Default: source at surface;
if source in focus at Z>0, thus INSIDE the layer system: add 1000 to phi)

if RING-shaped beam:
enter MAX.ring radius + 1000 [mm] in stead of theta,
and MIN.ring radius [mm] in stead of phi.
(Rectang. distr. only!)

FOCUS:

- > Z-position of focus with respect to sample surface [mm] (-1000 for // beam)
(Optional: X,Y-pos. of focus [mm]: at same line with Z-pos., ==>
format: (e.g.) -3.32/1.245/-0.27 for Z/X/Y-pos. Watch the sequence !!)
NB. If focus.Z=-1000, then // beam perpendicular to surface, independent of
tilting angles!.
If you like // beam, // tilting direction: take focus.Z=-999.99.

> DIAPHRAGM radius of beam at sample surface (*+1: circle; *-1: square) [mm]

> REFRACTIVE INDEX of the medium in front of the system of layers

> Id. of the medium behind the system of layers

-
-

> ** NUMBER OF TYPES OF SCATTERERS, LAYERS AND objects **

> Number of Types of scatterers

NB. Different types differ in RELATIVE Refr.index (w.r.t medium)
and/or Aspect ratio (circumference/wavelength)
and/or Mie-file (scattering function) !!

> Number of Layers

> Number of Objects

> Directory (folder) where the *.MIE-files are located.

-
-

FOR EACH TYPE OF SCATTERER :

>> ** SCATTERER # ** (#: nr.)

>> SCATTERING TABLE (*.MIE-file name, without extension .MIE)

This table must have been created in advance of the simulations!
For layers or objects without a predefined concentration or sigma_scatt
[um²] but with a known mu_scatt [mm⁻¹], relat.refract.index and
phase (or scattering) function of the particles, the PROCEDURE is:
: create the proper Mie-file using the rel.refr.index by adjusting the
aspect ratio at the proper wavelength;

: insert this Mie-file in the *.INP-file and adjust the concentration

>> ABSORPTION CROSS SECTION (sigma_absorption) [um²] of these particles.

In case the absorption coefficient (mu_abs) [mm⁻¹] of these particles
is known, adjust sigma_abs [um²] using the concentration found above

until the right `mu_abs`-value is reached.
The `mu_abs` of the layer as-such can be inserted also (see below) !

REPEAT this input for all other types of scatterers!

- - - - -

FOR EACH LAYER AND OBJECT [First all layers, then all objects]
[ALL entries on separate lines !!!]
[All dimensions etc. in mm !!!]

CONVENTION for the numbering of objects:

objects may be nested (wholly or partially) within each other.

To determine what properties will be valid in the region of intersection,
the rule is that there the properties of the object with the LOWEST
number will be used.

Example: two overlapping spheres 1 and 2,
with radii (1) 5.0 mm and (2) 4.0 mm:
in the region of intersection the properties of (1) will be used.

==> Following data have to be entered for each layer and object,
each on a separate line <==

>> ** LAYER # ** OR ** OBJECT # ** (#: nr.)

>> (if object) : TYPE of object:

B: rectangular, S: spherical, C: conical,
R: random spheres in a cylindrical volume (axis // Z-axis),
M: mirror plane, or: X,Y,Z: cylindrical, in x,y,z-direction,
T: half-torus in xz-plane, symm.axis // Y-axis,
L: lens (thick or thin; symm. axis // Z-axis).

=> IMPORTANT: A change in refractive index of the layer (or object)
will affect the scatt.cross section (`sigma_scatt` [μm^2]) of the
particles in it, because the local wavelength will change.
Since the program calculates the scattering coefficient `mu_scatt`
[mm^{-1}] from the cross section [μm^2] * concentration [mm^{-3}],
the scattering coefficient will be affected also.
You may stick to the "old" value for the scatt.coefficient
by correcting the concentration.

FOR EACH TYPE OF SCATTERER IN THIS LAYER OR object:

>>> CONCENTRATION [in 10^6 per mm^3]
>>> (if conc.<>0) : VELOCITY [mm/s]
>>> (if conc.<>0 and velocity<>0) :
> DIRECTION: X,Y,Z or R (R=random) or Q (= along axis of Q-object)
> TYPE: Uniform/Poiseuille/Gaussian (enter: U/P/ or 0..9) (see below)

FOR EACH LAYER OR OBJECT (continuing):

>> REFRACTIVE INDEX of the layer or object (= the medium for the particles;
if Mirror with 100 % -reflection: enter: 10000).
>> ABSORPTION COEFFICIENT `mu_abs` [mm^{-1}] of the material of
The layer or object.
>> (if layer): THICKNESS [mm]
>> (all objects, except L): no. of HIGHEST layer, in which
the object extends;
>> (if B-object): dimensions: Xmin, Xmax, Ymin, Ymax, Zmin, Zmax [mm];


```

>> (if X,Y,Z,M,Q,R,C-object): nr. of DEEPEST LAYER, in which the object
extends;
>> (if X,Y,Z,M,Q,S,C,T-object): X, Y and Z-coord. of a point on the axis
[mm];
>> (if X,Y,Z,Q,S,C,T-object): inner radius [mm];
>> (if X,Y,Z,S,C,T-object): repetition distance between objects [mm];
>> (if M,Q-object): direction angles: theta and phi [degr.];
      with theta and phi = polar (with Z-axis and azimuthal (with X-axis)
      angles. NB. Pos. Z-axis points INWARD layer system !
>> (if R-object): random spheres in a cylindrical volume:
  >> X and Y-coord. of a point on the cylinder axis;
      (NB. the cylinder will stretch over the whole of the layer(s) it is
in!)
  >> concentration [# spheres/mm^3];
  >> average sphere radius [mm] and cylinder radius [mm];
  >> standard deviation of sphere radii [mm];
  >> overlap of spheres allowed? Y/N;
>> (if T-object): (NB. T-object = half torus!)
  >> Direction of U-shaped opening of half torus:
      towards +Z (enter: +1) or -Z (enter: =-1).
      (NB. Torus MUST be completely located in 1 (one) layer;
      so: no extension across layer boundaries!!)
>> (if Z,Q,T-object): INNER WALL = specular reflecting (mirror) or absorbing:
      add "100" or "200" resp. to the value of the max.layer nr.
>> (if C-object): Bottom-to-top direction:
      +Z,-Z,+X,-X,+Y,-Y: enter: 1,2,3,4,5,6 resp.
>> (if L-object):
  >> X- and Y-positions of symmetry axis;
  >> Z-positions of intersections of front and back surfaces with
symm.axis;
  >> radii of curvature, front and back (pos/neg if behind/in front of
lens);
  >> diameter (perpendicular to symm.axis);

```

> ** CALCULATION MODES & DETECTION **

```

> = CALCULATION MODES: OPTIONS:  [<...> = averaged over photons] : Enter:
S:   Reflection:   store <scatt.depths> and max.photon.depth;
R:   Reflection:   store <scatt.depths> and <Dopp1.scatt.depths>;
T:   Transmission: store: as with R;
I,J,K: Internal:   store depth of detection and max.photon.depth,
      = detect at passage (in->out) of a sphere surface
      or a curved surface of a cylindrical tube or cone;
      I = all; J/K = at reflection/transmission side;
A:   Absorption:   store depth of absorption and max.photon.depth;
E:   All:          = S+T+A (<version 2018: R+T+A);
Additionally with all options:
      store positions immediately after N-th flight-time step
      (see below, with N>0 and flight time step size dt>0).
Extra option:
D:   Duration:     photon terminated immediately after (N+1)th time
step.

```

```

= (Optional) PATH LENGTHS: Geometrical=default. Optical? Add: 0.
= (Optional) FLIGHT TIME POSITIONS : (see also in chapter 15.)

```

If storage of flight time positions wanted: add nr. of time steps N (max N=9) and time step size dt (in sec.) on the same line with S/R/A/T/D/E:

FORMAT (keep exact!!) (e.g.): if you want:

Reflection S, max.depth, and optical path lengths,
with N=5 and dt=1.2E-15 sec: --> enter: S0+5x1.2E-15

NB. If CALCULATION MODE = D (Duration) then *.FOx-file (x=0..9) contains time-of-flight positions after (N+1)-th time step, thus NOT at time of detection or absorption.

NB. If CALCULATION MODE = I,J,K (Internal detection at a SPHERE surface or curved surface of a CYLINDER or a CONE), the program automatically stores the detection positions in rectangular coordinates. However, for SPHERES and CYLINDERS the program offers optional recalculation of the X,Y and Z-positions of photons at their detection position into:
- polar angle theta (w.r.t. local Z'-axis through sphere center)
- azimuthal angle phi (w.r.t. local X'-axis)
This option is available when plotting or with Ascii-output of the photons.

I = all;

J = photons, internally detected at reflection side only

K = id. ... at transmission side.

- - - - -

DETECTION FIELD AND NUMERICAL APERTURE OF DETECTORS

DETECTION FIELD [mm]:

> Min.Xfield, max.Xfield, min.Yfield, max.Yfield [on 4 separate lines].

(NB: for 2- and 3-dim storage, this field will be divided in 20x20 pixels in the X- and Y-direction.

In the "scattering" mode a detector with arbitrary dimensions may be placed in this field; division in 20 pixels.)

In case you want ring-shaped detectors:

consider Xfield as Rfield, and insert min.Yfield=max.Yfield=0; then min.Xfield<max.Xfield is necessary! otherwise: no width!

In case of absorption followed by fluorescence/Raman:

use identical detection fields in both cases!!

> (on one line!:) NUMERICAL APERTURE (NA) of detector (IN VACUO !!) + REFRACTIVE INDEX OF DETECTOR SURFACE; (format example: see below.)

NA = sin(th), with th = half opening angle ($0 < th \leq 90$ degr.); (completely open: NA = 1)

- In case of reflection and detection at interface of layers

N and N+1: (NB. surface: N=0) : -> add N*10 to NA.

- In case of internal detection upon passage of the curved surface of a sphere, cone, torus or cylinder : -> add object.nr*10 to NA

EXAMPLES OF INSERT FORMAT :

with NA=0.73 and refr.index of detector = 1.58:

- for detection at surface (layer 0) -> enter: 0.73/1.58

- for detection at interface of layers 2 and 3 -> enter: 2.73/1.58

- for detection in object 3 -> enter: 3.73/1.58

- if Calculation mode = T (transmission) -> enter 0.73/1.58.

> ** DEPTH PIXELS **

Each layer may be divided into depth pixels. Min. 1 pixel/layer.
Useful for 2D/3D-output files.

> For each layer: enter nr. of pixels [on separate lines]

```
File: C:\WC\Eenlaah1.FOT
Screen borders Min: X: -10.000 | Y: -10.000 | Z: 0.000 mm
                  Max: X: 10.000 | Y: 10.000 | Z: 6.000 mm
75 paths plotted: ready.
```

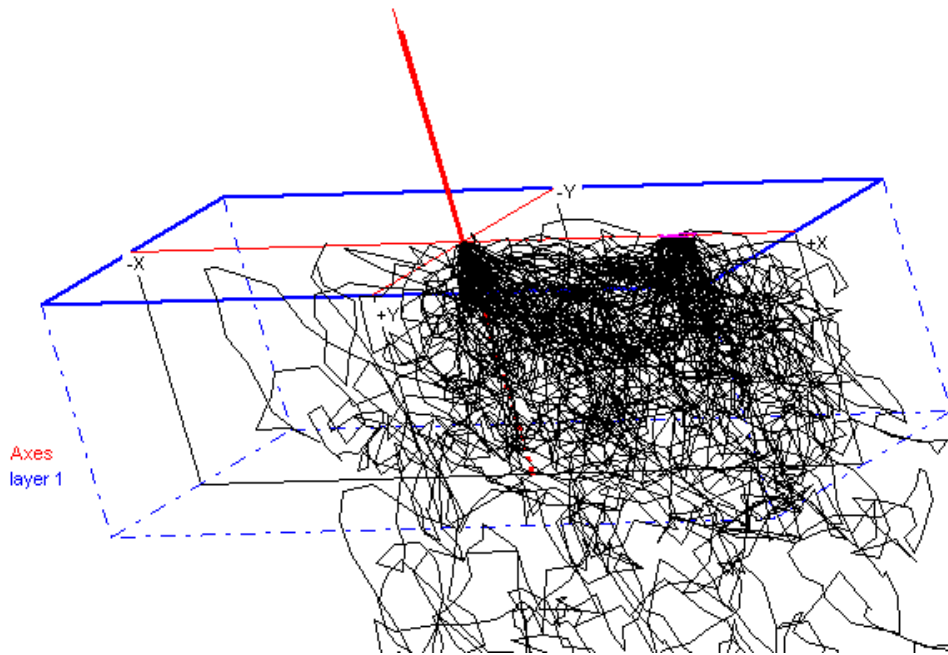


Fig.6. Photon path tracking: Photon “bananas” arising by scattering from beam entrance point to exit area (between 5 and 6 mm). For clarity, all photon paths were rotated afterwards as if the photons had emerged on the +X-axis.

> ** FILE OUTPUT **

(NB. The output files will have the same name as the *.INP input file)

> DIRECTORY (FOLDER) to store the output files.

> STORE : *.FOT-file(s) (enter F), *.2D/3D-files (enter D) or both (enter B)
(only if PATH TRACKING wanted; otherwise skip): Add to F/D or B:

A: Store positions of all scattering events (+reflections/refractions);
this option means spacing of about $1/\mu_s$;

R: Store # scatt.events * (1-g) (+refl./refr.);
this option means spacing of about $1/\mu_s'$ with $\mu_s' = \mu_s * (1-g)$;

example: this line should read e.g.: FA or F or BR or B or

> (only if Store = D or B :) Linear/Quadratic XY-PIXELS in 2D/3D-files:
enter L/Q

> ** NR. OF PHOTONS **

NB. The number of photons is only restricted through the available space in the output directory.

However, when analyzing the data with this program, the number of photons may be restricted due to the available RAM-space.

The 2- and 3-dim-files contain information of ALL photons.

To CHANGE nr. of photons DURING simulation:

- Interrupt simulation using "Interrupt"-button;
 - change Nr. of photons in *.INP-file;
 - Resume simulation
- > NUMBER OF PHOTONS, to be : either:
- emitted by the source (enter E),
 - injected in the sample (enter I),
 - accumulated in the detection window (enter D),
- Enter: E,I, or D, followed by the number, on same line (e.g.: D100000).
 NB. With fluorescence/Raman:
 if D chosen, and the nr. of absorbed FOT-photons is not sufficient,
 the absorption FOT-file is used repeatedly (at start
 the photons will have different directions compared with previous use).
- > (only if moving scatterers present; otherwise skip):
 Store DOPPLER-SHIFTED photons only? Enter Y/N

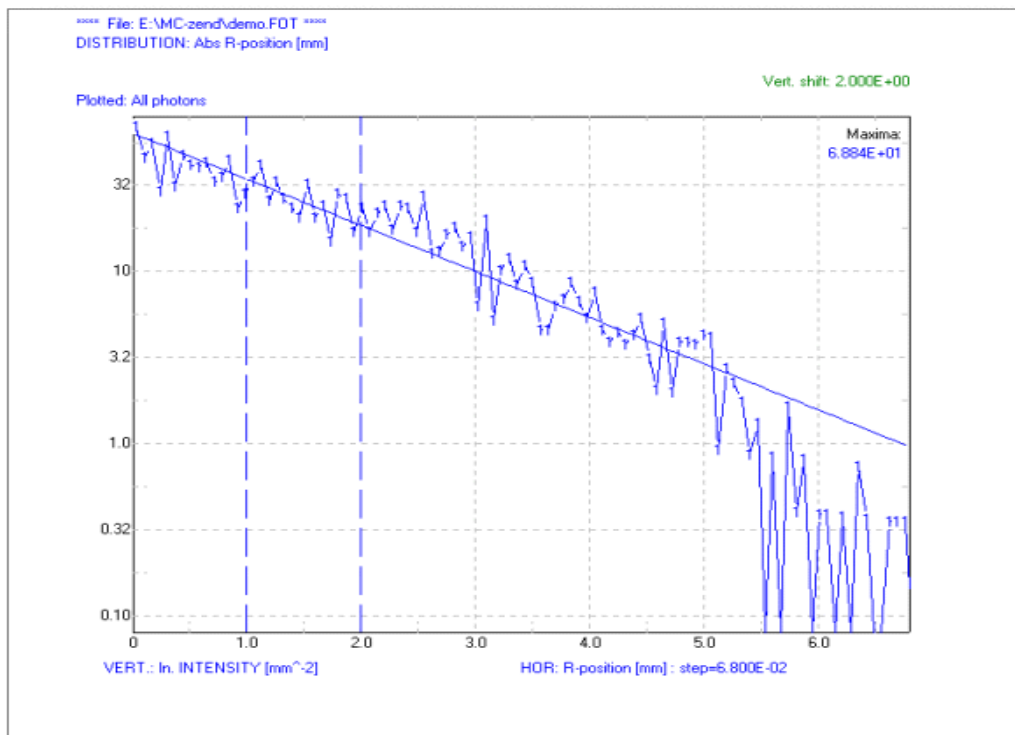


Fig.7. Example of output plots. Here \ln (Intensity) vs. R-position from the Z-axis. Also included: a model approximation (solid line)

==== 14. VELOCITIES : profiles and distributions ====

Options: (in all cases: velocity to be entered = $\langle v \rangle$!!)

- Uniform: all velocities of the present scatterer in the present layer or object have the same magnitude;
- Poiseuille: a parabolic profile, extending to the layer or object boundaries (where $v=0$):
 - = layer with flow in X or Y-direction; (depth variable: d ; thickness D):
 $v(d) = v_{\max} \cdot [1 - d^2/(D/2)^2]$;
 $v_{\max} = 3/2 * \langle v \rangle$; ($v_{\max} = v$ on *symm.axis*)
 if flow in Z-direction: treated similar, with $z =$ variable;
 - = tube: cylinder: (variable: r ; radius R):
 $v(r) = v_{\max} \cdot [1 - (r/R)^2]$; $v_{\max} = 2 * \langle v \rangle$;

torus: similar, flow always parallel to (curved) axis;
 = block (rectangular): approximated as N-dimensional parabolic profile,
 e.g. if flow in X-direction: 2 distributions (N=2)
 with variables y and z:

$$v(y,z) = v_{\max} \cdot [1 - y^2/(Y/2)^2] \cdot [1 - z^2/(Z/2)^2],$$
 with Y and Z the dimensions.

$$v_{\max} = (3/2)^N \cdot \langle v \rangle,$$
 with N=2; if random direction: N=3.
 - Gaussian: Gaussian profile, e.g. for Brownian motion;
 sigma is expressed in N * 5 % of $\langle v \rangle$, with N=0..9;
 N to be entered in the input file.
 NB. Objects of type R,S,L (spheres or lenses): only random directions.

==== 15. PHOTON DATA STORAGE in *.FOT AND *.PAT-files : ====

*.FOT (F0x)-files:

For each photon the following data are stored (24 bytes/photon):

- {Ri/Ii: Real/Integer; i=nr. of bytes}: (*)= see below: COORD. UNITS
 - I2: X-coord. of point of detection or absorption [unit: 1 or 10 um]; (*)
 - I2: Y- [id.]; (*)
 - I2: either: average depth of all scatter events; or :
 maximum depth, or: point of detection or absorption [id.];
 - I2: id. of all Doppler scatter events [id.];
 - R4: path length [mm];
 - R4: Doppler frequency [Hz]; ==> (*): see below <==
 - I4: number of scatter events;
 - I1: percentage of Doppler scatter events;
 - I1: theta: angle with pos.Z-axis (!) at detection or absorption [deg] (*)
 - I2: phi: angle with projection of vector on XY-plane with X-axis [deg] (*)
- Convention: : theta : phi :
- reflection : 180 >= .. >= 90 : 0 <= .. < 360 :
 - transmission : 90 >= .. >= 0 : 0 <= .. < 360 :
 - absorption : 180 >= .. >= 0 : 0 <= .. < 360 (o) :
- (o) stored in *.FOT-files as: -phi-1 . ==> (*): see below <==

The photons are stored in the *.FOT-file in bunches of 1000.

(*) COORDINATE UNITS

For program versions < 2018:

The X-,Y-coordinates are stored as "integers", and the depth-coordinates as words" in units of 1 (default) or 10 micrometer;

The 10 micron-unit is used:

- for XY-coordinates: in case the XY-detection field extends beyond +/- 32.767 mm (= 32767 micron = max. |smallint| value);
- for Z-coordinates: in case the layer system thickness > 65.535 mm (= 2 x 32767 micron = max. word value)
 (smallint: 2 bytes: -32768..+32767; word: 2 bytes: 0..65535)

For program versions >= 2018:

The X-,Y-coordinates and the depth-coordinates are stored as "singles", 4 bytes each, with no size limitations;

PATH CROSSINGS [%] | -3.000 < length < 3.000 | 0.000 < width/depth < 2.000 | All photons
 Values: 100 % = 2.340E+02 in plane: 5 ; this screen max = 5.600E+01

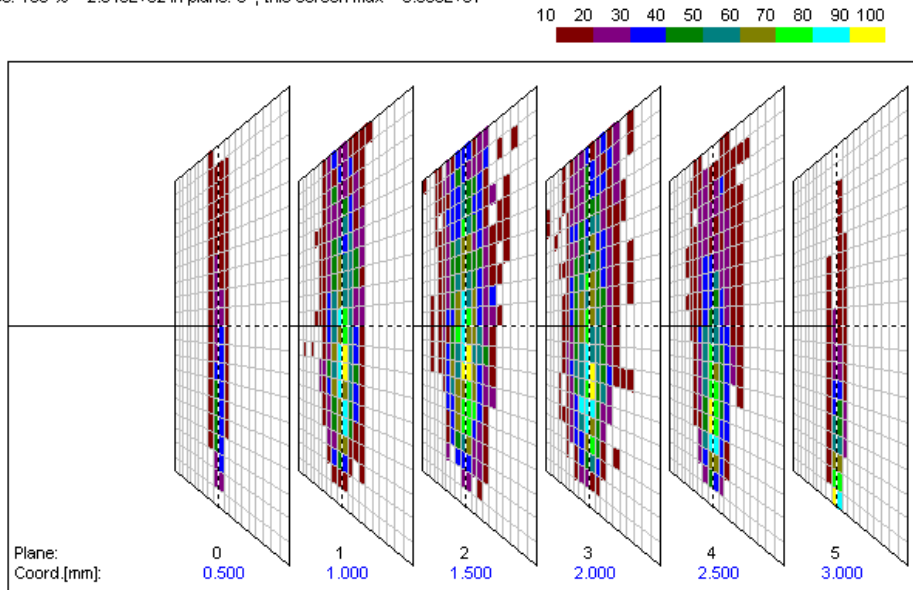


Fig.8. 3D-plot of Path tracking: photon “bananas”: average depths of photon paths. Entrance at position 0; photons emerging between positions 5 and 6 mm from entrance.

In case of INTERNAL DETECTION (calculation mode= I,J,K):

The POSITION coordinates of the point-of-detection are stored as follows:

- : X-, Y- and Z-coordinates on layer system axes;
- : and the depth-coordinate as above, all in integer format;

In case of recalculation from Cartesian into angular coordinates (see above) here the polar axis is the local Z'-axis (// Z-axis) through the sphere center or the symmetry axis of the cylinder or cone , and the azimuthal angle is measured from the local X'-axis (// X-axis).

The DIRECTIONAL theta and phi, otherwise measured as mentioned above, now are measured from the local coordinate system in the detection point (local Z"-axis = polar axis = normal through sphere center, and local X"- and Y"-axis = south-north and east-west direction on sphere).

FLIGHT TIME POSITIONS:

Detected photons can be followed during flight; stored in *.FOx files, with x=0..9 time steps, with time-step size to be inserted in the *.INP-file.

*.FOx files have same format as *.FOT-files.

Using the option: "View structure of layer system" the evolution of the photon density can be followed on-screen. n.

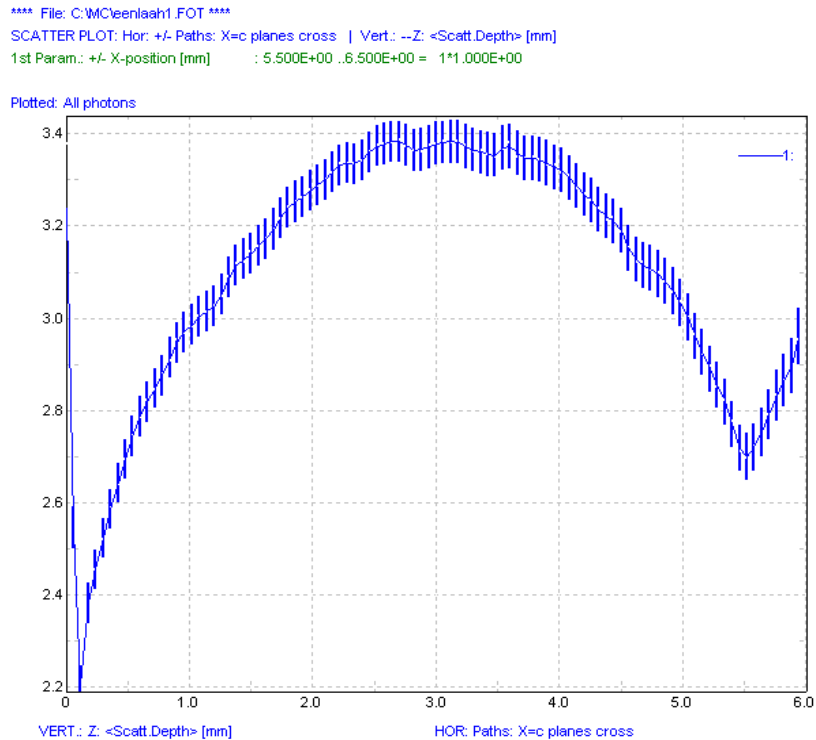


Fig. 9. Paths tracking: Averaged depths of photons, with standard deviation in the average. Settings: see fig. 5. Plot for distance > 5.5 mm is due to spurious photons.

PATH TRACKING : PHOTON PATHS STORAGE IN *.PAT-FILES (path tracking)

Only paths of detected photons are written in the file.
 The *.PAT-files have similar format for x,y and z-data as the *.FOT-files.
 This means that each path position is written as:
 "smallint, smallint, word" for x,y, and z respectively (see above).
 Each photon path is written as follows:
 - leader: x=9999, y=9999, z=N, with N = nr. of events to follow
 (scattering/reflection/refraction)
 - for each of N events: x, y and z-value (in units as mentioned above).

==== 16. AVERAGED DATA : in pixels in detection field ====

In order to have data about all photons available, averaged data may be stored in *.2D and *.3D files, in which 2- and 3-dimensional pixels are filled during the calculations.
 The horizontal (X and Y) pixels are defined as amounting to 1/20 of the dimensions of the detection field; the vertical (Z) pixels have to be entered in the *.INP file separately (see below).

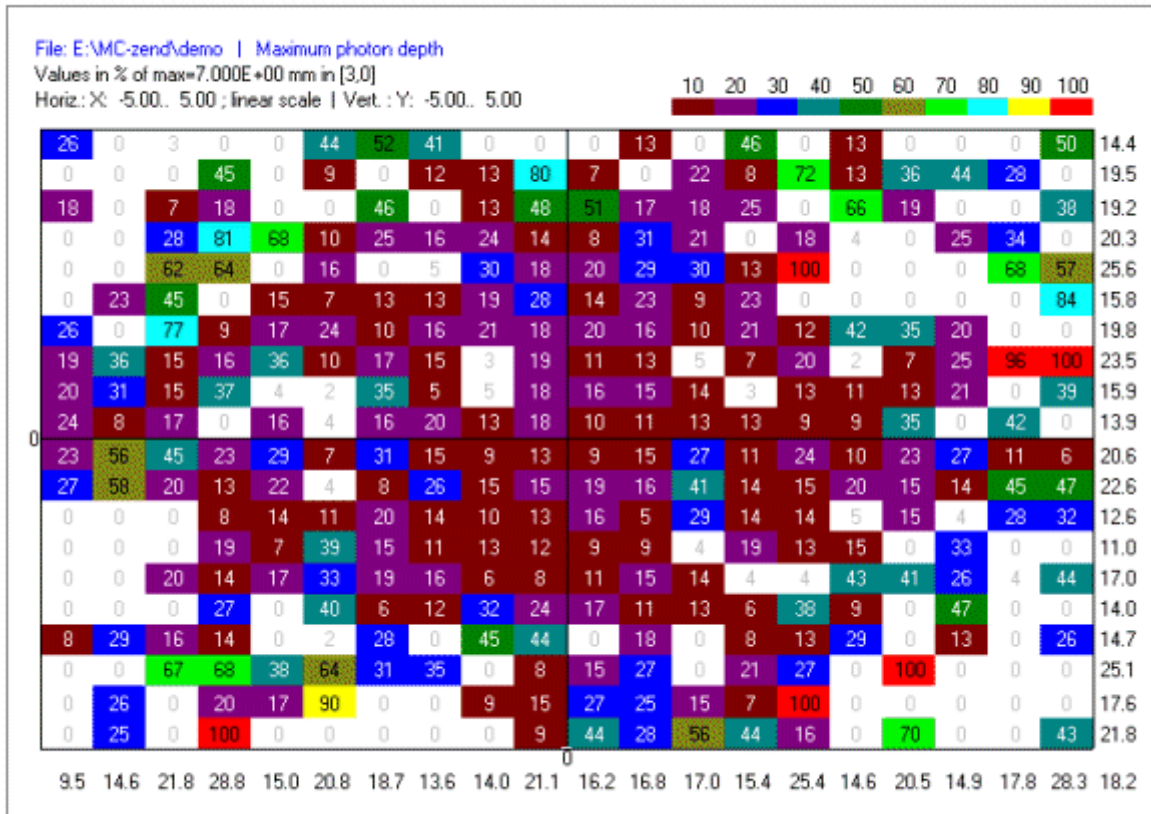


Fig.10. Example of 2D-plot: Here the maximum photon depth plotted as function of (x,y)-positio

==== 17. INTENSITY APPROXIMATIONS : I(r) (r= source-detector distance) ====

The Option "Results" + "Distributions" + "Hor.Var.= r"

offers the possibility to fit some analytic intensity models to the simulated intensity distribution.

The models are:

- $I(r) = c1 * \exp(-c2*r) / r^x$, with $x = 0, 0.5, 1$ or 2 .

- $I(r)$ = according to the Farrell-model (with 1 source).

Here the constants are:

- $c2 = \mu_{eff} = \sqrt{3 * \mu_a * (\mu_a + \mu_s')}$, with $\mu_s' = \mu_s * (1-g)$;
 (μ_a, μ_s = absorption and scattering coefficient in 1/mm;

μ_s' = reduced scatt.coeff.; g = anisotropy factor);

- $c1 = \text{power} * \mu_{eff}^2 / (4 * \pi * \mu_a)$, with power = nr. injected photons;
 (NB. this expression for $c1$ is valid for $x=1$ only !)

The Farrell model is:

$I(r) = \text{albedo} * \text{power} / (4 * \pi) * [z01 * (\mu_{eff} + 1/r1) * \exp(-\mu_{eff} * r1) / r1^2 + z02 * (\mu_{eff} + 1/r2) * \exp(-\mu_{eff} * r2) / r2^2]$,

with $z01 = 3D$; $D = 1 / (3 * (\mu_a + \mu_s'))$; $z02 = z01 + 4AD$;

$r1^2 = z01^2 + r^2$; $r2^2 = z02^2 + r^2$; $\text{albedo} = \mu_s' / (\mu_a + \mu_s')$

A = Fresnel correction: $A = (1+ri) / (1-ri)$;

$ri = 0.668 + 0.0636 * n + 0.7099 / n - 1.4399 / n^2$;

n = relative refract.index from scattering medium to detector medium.

Output: $c1$ and $c2$, or (for Farrell) μ_a and μ_{eff} , resulting chi-squared.

NB. The circular integral (CI) over the Farrell-distribution:

CI = $\int_0^{\infty} I(r) \cdot 2 \cdot \pi \cdot r \cdot dr$, gives:

= $\text{albedo}/2 \cdot \text{power} \cdot \exp(-\text{del}) \cdot [1 + \exp(-4A \cdot \text{del}/3)]$, with $\text{del} = \mu_{\text{eff}} \cdot z_{01}$;

If "power" = # injected photons, then CI should be = # reflected photons.

==== 18. PHOTOACOUSTICS : DETAILS ====

The program calculates the PA-RESPONSE on the basis of a spherical source with dimensions of an absorption voxel. This implies a bipolar shape, given by : $(c^3) \cdot k \cdot \exp[-(ck)^2]$, with $k = (i - i_0) \cdot dt$, $(i - i_0) \cdot dt$ is the time difference to the time point of the zero-crossing (at $i_0 \cdot dt$) of the bipolar shape, $i = \text{nr. time steps}$. The constant c is: $c = 1/[\text{sqrt}(2) \cdot \text{sigma}] = 1/\text{tau}_e$, and sigma (or tau_e) is the characteristic width (see: TIME REGIME). This bipolar shape is then multiplied by:

(1) $\exp(-\mu_{\text{att}} \cdot r) / r$,

where r = the distance from absorption voxel to detection pixel, and μ_{att} is the ultrasound attenuation coefficient (averaged over the frequency band of the acoustic signal),

(2) the area of a detector element [mm^2].

TIME REGIME:

Here the time window (nr. of time elements i and element size dt) can be inserted. The time-of-flights to be calculated are: perpendicular and diagonally through the (reduced) absorption volume. A measure for the PA pulse width is tau_e : the "effective pulse length", given by the laser pulse HWHM and the transit time of the acoustic pulse through the elementary source ("radius" = $Z\text{-vox.}/2$).

$\text{tau}_e = \text{sqrt} [\text{HWHM}^2 + (Z\text{-vox.}/2/\text{sound.velocity})^2]$.

which defines sigma : $\text{tau}_e = \text{sigma} \cdot \text{sqrt}(2)$.

The peak-peak time (from pos. to neg. peak) = $2 \cdot \text{sigma}$.

We take i_0 to begin at $3 \cdot \text{sigma}$ before the zero-crossing of the signal.

The starting time of the sound recording can be shifted, in order to avoid time regions where no signal is expected.

GROUPING OF DETECTORS:

The PA-response is calculated for each detector at its center point. This means that no interference of sound waves over the surface is taken into account. To do that properly, it is advised to use small detector elements and GROUP those into X- and Y-groups. In doing so, probable interference is calculated automatically.

Each group MUST consist of an integer nr. of detector elements.

DIRECTIVITY OF DETECTORS:

Each detector "looks approximately forward" from its center point into the absorption field of voxels,

but can be given a NUMERICAL APERTURE (called "directivity").

Directivity correction: relative w.r.t. 0 degrees;

- available types: U: Uniform, G; Gaussian, T: triangular;

- HWHM (half-width at half-maximum to be entered in degrees.

(normalisation: sensitivity = 1 for perpendicular view (0 degr))

*** PHOTO-ACOUSTIC RESPONSE ; File: ABS19141 ***

Plot normalized on absolute maximum: 1.403E-05

Signal: Min: -1.161E-05 Max: 1.403E-05

Time window: -53.3.. 3000.0 = 3053.3 ns ; start shift: 0.0 ns

Depth : 0.080.. 4.500 = 4.580 mm ; 0.000 mm

Detectors : (X,Y)-groups: (1,1) ...(7,7)

... X-positions: -5.000 .. 5.000 mm ; 0.400 mm/det

... Y-positions: -5.000 .. 5.000 mm ; 0.400 mm/det

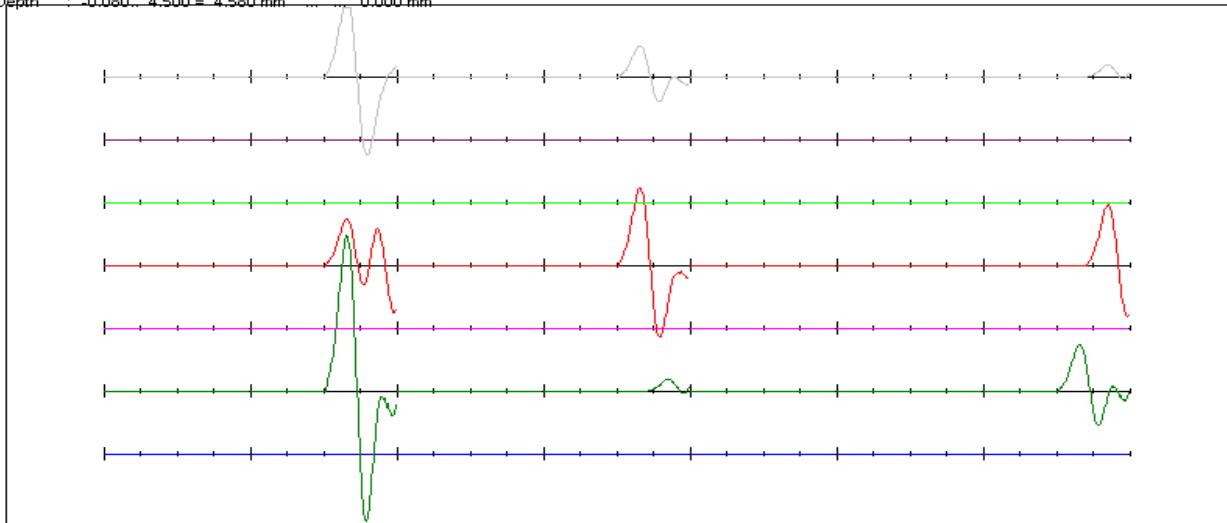


Fig. 11. Photoacoustic response at a 7 x 7 - detector array of a sample consisting of several absorbing objects in a scattering (but not absorbing) medium.

==== 19. FREQUENCY-MODULATED PHOTON SOURCE ====

Normally the photons are injected as a delta-pulse in time, all at $t=0$.

The path length distribution is similar to the time-of-flight distribution;

the prop.factor is $1/\text{light velocity}$.

The program has two options for recording the paths:

(a) geometrical or (b) optical.

In (a) the prop.factor is taken as $1/\text{light velocity}$ in the 1st layer;

in (b) the optical path = geometrical path / local refractive index;

therefore here the prop.factor = $1/\text{light velocity on vacuo}$.

However, the photons could also be injected using a frequency-modulated light source, with typical frequencies of 100 MHz - 2 GHz. Then the frequency response is the Fourier transform of the time-of-flight distribution upon the pulse input.

The plot output offers options for plot of the phase delay (in degr.) and the modulation depth (dim.less), defined as:

$$\text{phase delay}(n) = \arctan \{ \text{Im}[f(n)]/\text{Re}[f(n)] \} ,$$

$$\text{modulation depth} = \sqrt{\text{Im}^2[f(n)] + \text{Re}^2[f(n)]} / \sqrt{\text{Re}^2[f(0)]} ,$$

where $f(n)$ is the (Fast-) Fourier transform of the time-of-flight distribution.

If time step = dt , then max.freq. (f_{max}) = $1/(2*dt)$.

The freq.step df is $f_{\text{max}}/(N/2)$, where

N = nr of time steps in the time-of-flight distribution,

replenished up to a power of 2 (e.g. $N = 512, 1024, 2048$).

The program also offers the possibility to calculate the phase delay and modulation depth using analytic models published by:

- Haskell et al., for 1-layer samples,
- Kienle et al., for 2-layer samples.

References:

- R.C. Haskell et al., J.Opt.Soc.Am. A 11, oct 1994, p 2727-2741.
- A. Kienle et al., Appl.Optics 37, Feb 1998, 779-791.

==== 20. RUN TIME ERROR MESSAGES (from Borland Pascal) ====

1	Invalid function number	200	Division by zero
2	File not found	201	Range check error
3	Path not found	202	Stack overflow error
4	Too many open files	203	Heap overflow error
5	File access denied	204	Invalid pointer operation
6	Invalid file handle	205	Floating point overflow
12	Invalid file access code	206	Floating point underflow
15	Invalid drive number	207	Invalid floating point operation
16	Cannot remove current directory	210	Object not initialised
17	Cannot rename across drives	211	Call to abstract method
100	Disk read error	212	Stream registration error
101	Disk write error	213	Collection index out of range
102	File not assigned	214	Collection overflow error
103	File not open	215	Arithmetic overflow error
104	File not open for input	216	General protection fault
105	File not open for output		
106	Invalid numeric format		

Stub errors:

Stub error (0001) needs at least 286

Stub error (2002) can't find rtm.exe

Stub error (2003) can't find

DPMI16BI.OVL

Stub error (0012) file not found

Stub error (0013) path not found

Stub error (0015) file access denied

Stub error (0018) not enough memory to load file

Stub error (001A) invalid environment

Stub error (001B) invalid file

Error: no DOS extensions in the DPMI server

Error: needs DOS 3.x or higher

Error: failed to locate DPMI server (DPMI16BI.OVL)

==== 19. Contact address ====

The name of the help file is: MONTCARL.TXT (Ascii-format)

When in trouble, contact:

Dr. ir. F.F.M. de Mul,

e-mail: [ffm "at" demul.net](mailto:ffm@demul.net)

Previously: University of Twente, Department of Applied Physics,

Research Group: Biophysical Technology / Biomedical Optics,
P.O.Box 217, NL - 7500 AE Enschede, the Netherlands,

For regular updates of the program, see www.demul.net/frits

MORE FIGURES:

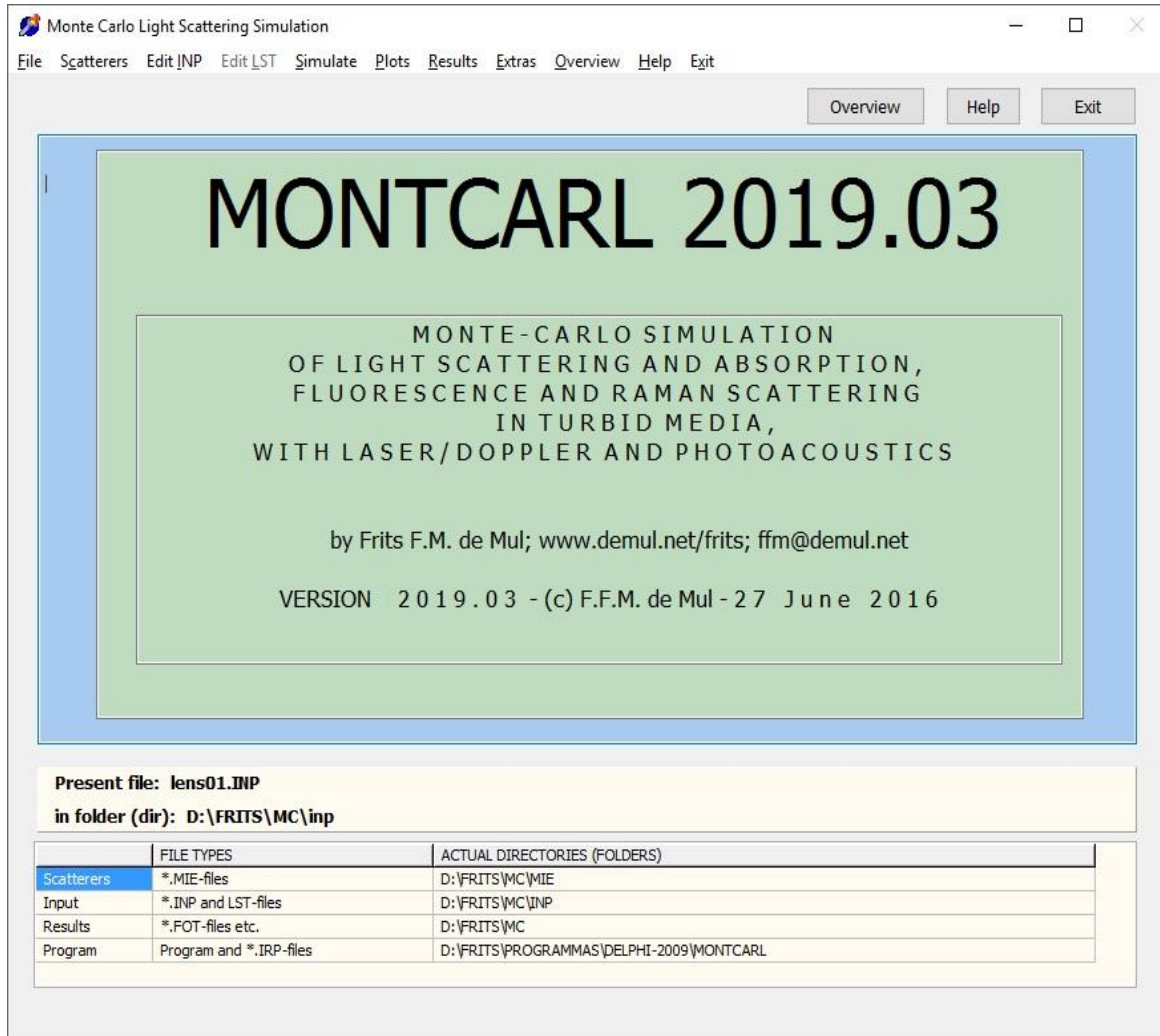


Fig. 12. Menu screen (with Tabs)

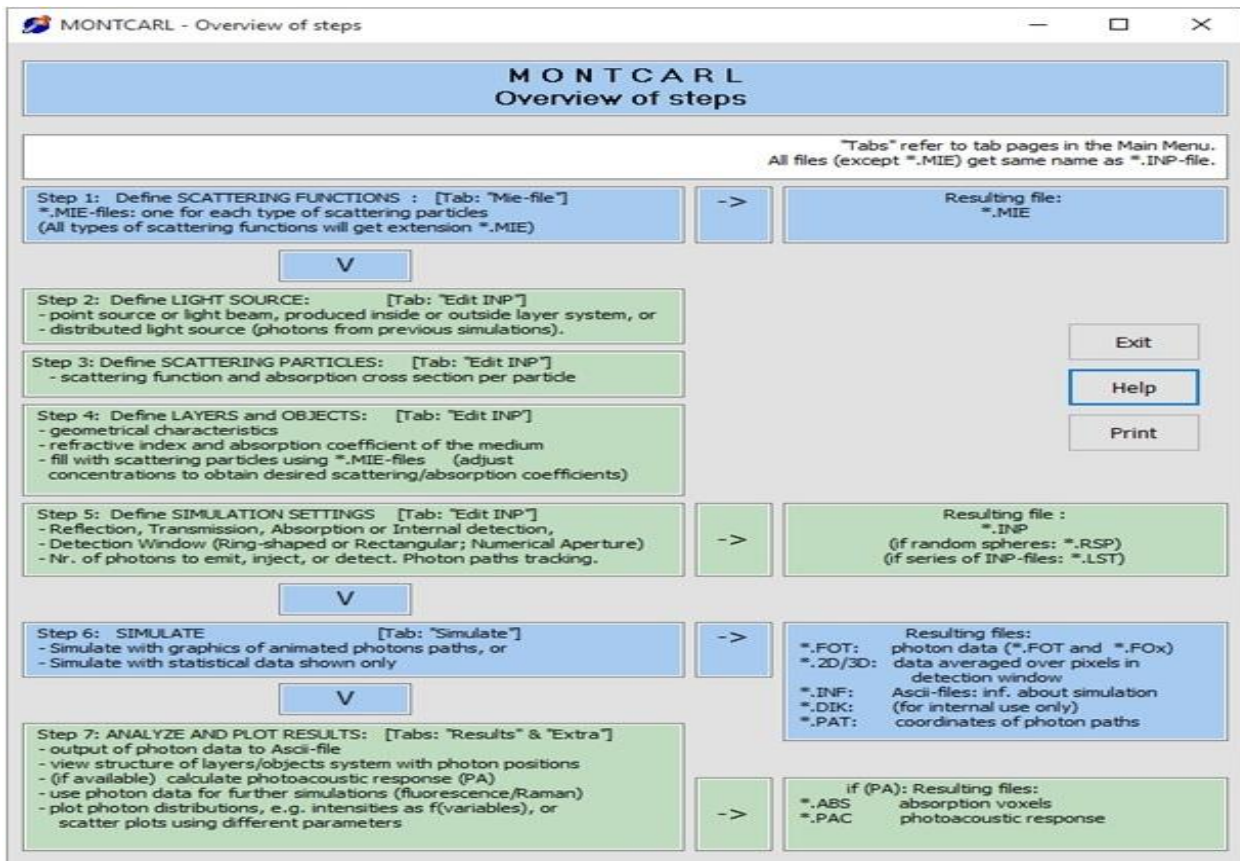


Fig. 13. Overview about how to input settings and to run simulations

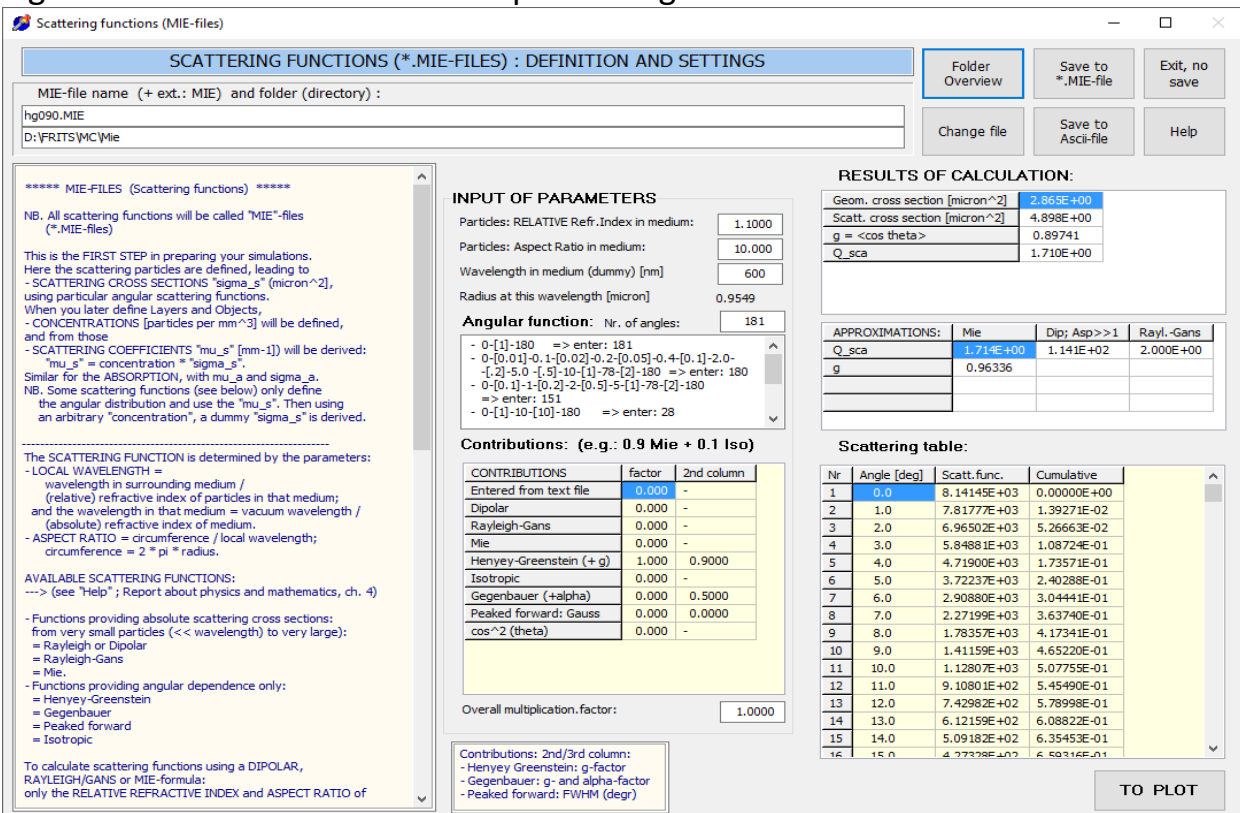


Fig. 14. Creation of scattering functions (called: *.MIE-files)

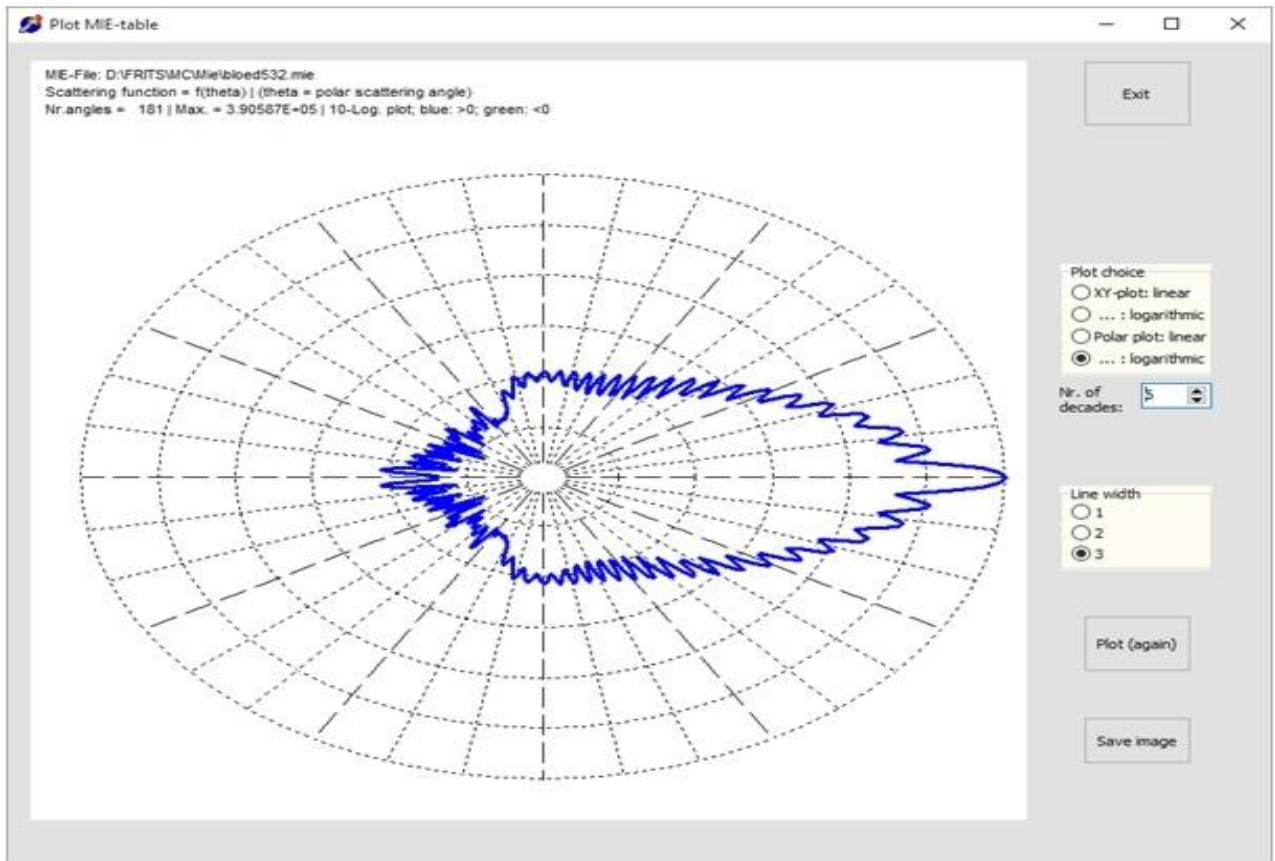


Fig.15. A scattering pattern (combination: Mie + Henyey-Greenstein-functions)

File: lens01
Directory of MIE-files: d:\frits\mc\mie

Directory Overview Add scatterer Remove nr: (0=exit) -1 Remove scatterer

INSERT for Scatterer no.: 1 Browse for MIE-file View MIE

Insert for each type of particle: the SCATTERING FILE (*.MIE) and ABSORPTION per particle will be changed in screen "Create/change MIE-file" in Menu-Tab: "Scattersers")

Scatterer:	1
MIE-file: (no extension!)	hg090
Absorption per particle [micr ²]:	0.000000

Refractive index of medium (dummy variable): 1.33 Wave

CALCULATED VALUES:

Rel.Refr. Index w.r.t. medium	1.100000
Aspect ratio in medium	10.00000
Q_scattering	1.709839
g = <cosine polar scat.angle>	0.897414
Particle: radius [micron]	0.957323
..geom.cross section [micr. ²]	2.879167
..scatt.cross section [micr. ²]	4.922912
..albedo = scatt/(scatt+abs)	1.000000

SELECTION OF SCATTERERS

In a previous screen (Menu Tab "Scattersers") you have created one or more "SCATTERING FUNCTIONS", in the form of *.MIE-files.

In this screen you will select which of these Scattering Functions you want to use in your layers and objects, for this particular simulation.

For that purpose: select the desired *.MIE-functions. See the buttons: "Directory Overview" and "Browse for MIE-file".

It is possible to add an ABSORPTION CROSS SECTION (in micr²) to the particles in the Scattering Function.

However, when you will arrive at the screens to define LAYERS and OBJECTS, it will be possible to define an ABSORPTION COEFFICIENT (in 1/mm) for the layer or object as a whole.

ABSORPTION: options:
(1) absorption of the particles (abs.cross section in micr²); and/or
(2) absorption in the medium of layer or object itself (abs.coeff. in 1/mm) :
(1) may be changed here;
(2) may be changed in the "Layers" or "Objects"-menu.
Coefficient = cross section * concentration (1/mm³)

Scattering- and absorption cross sections in layers and objects will be corrected from vacuum value (refr.index=1) to actual value by division by (refr.index)²

Fig.16. Selection of scattering functions for use in layers and objects

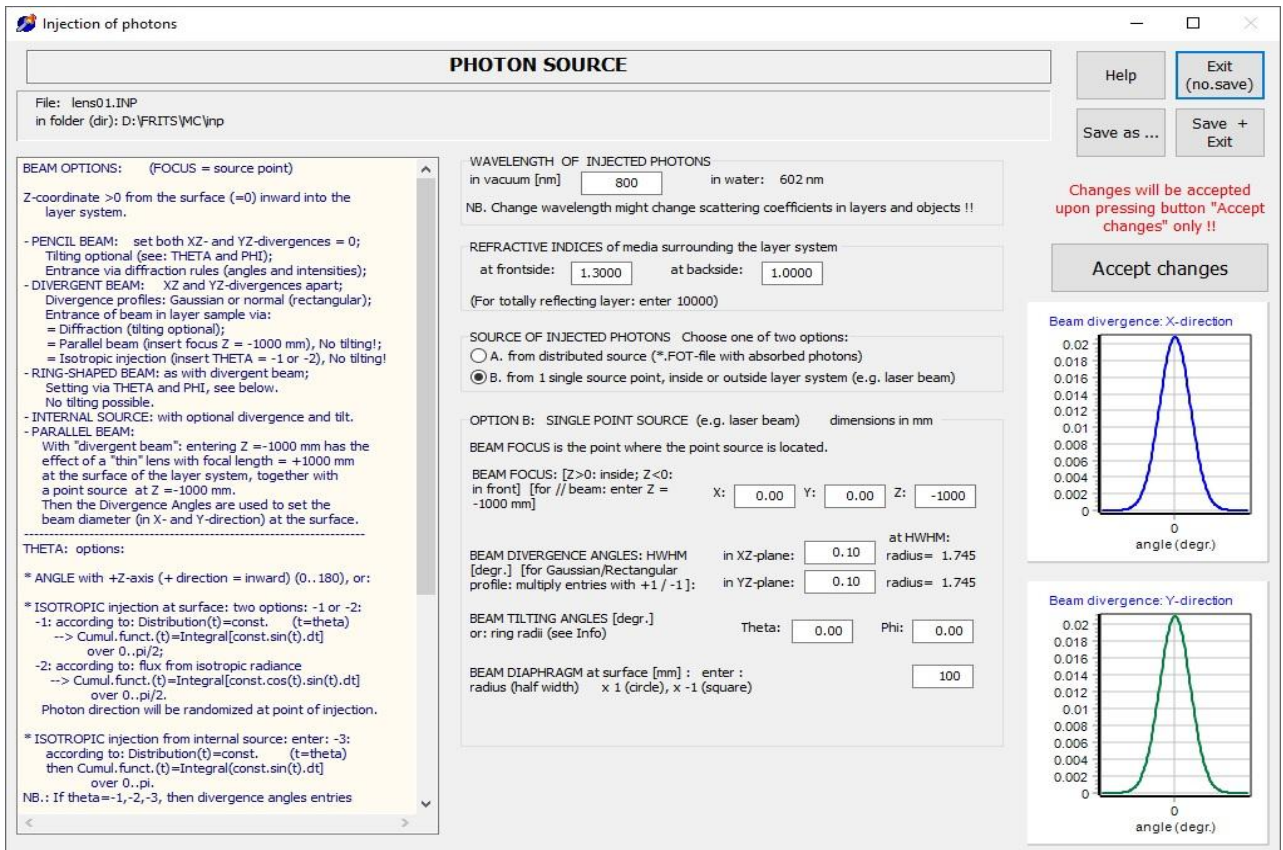


Fig.17. Input of data for the light source (e.g. laser data)

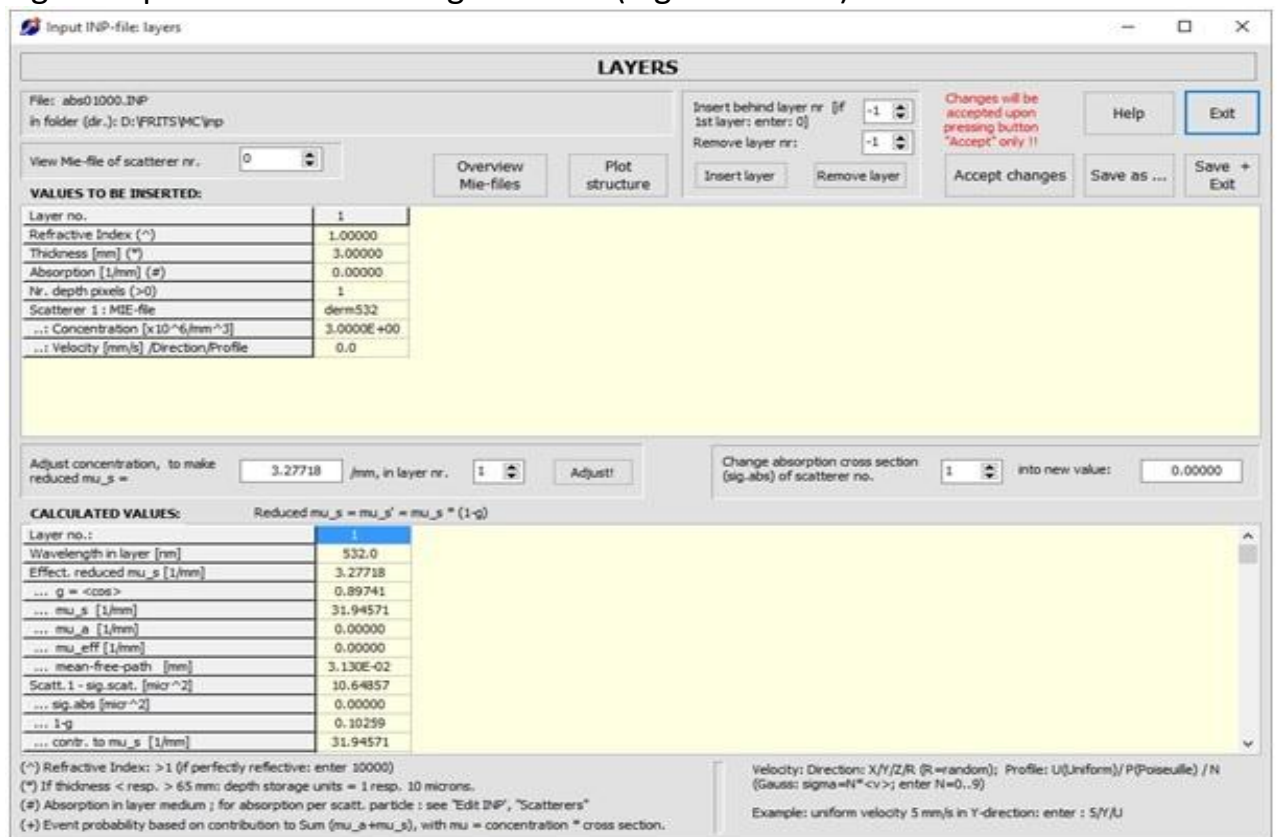


Fig. 18. Input of data for layers (more than 1 layer possible)

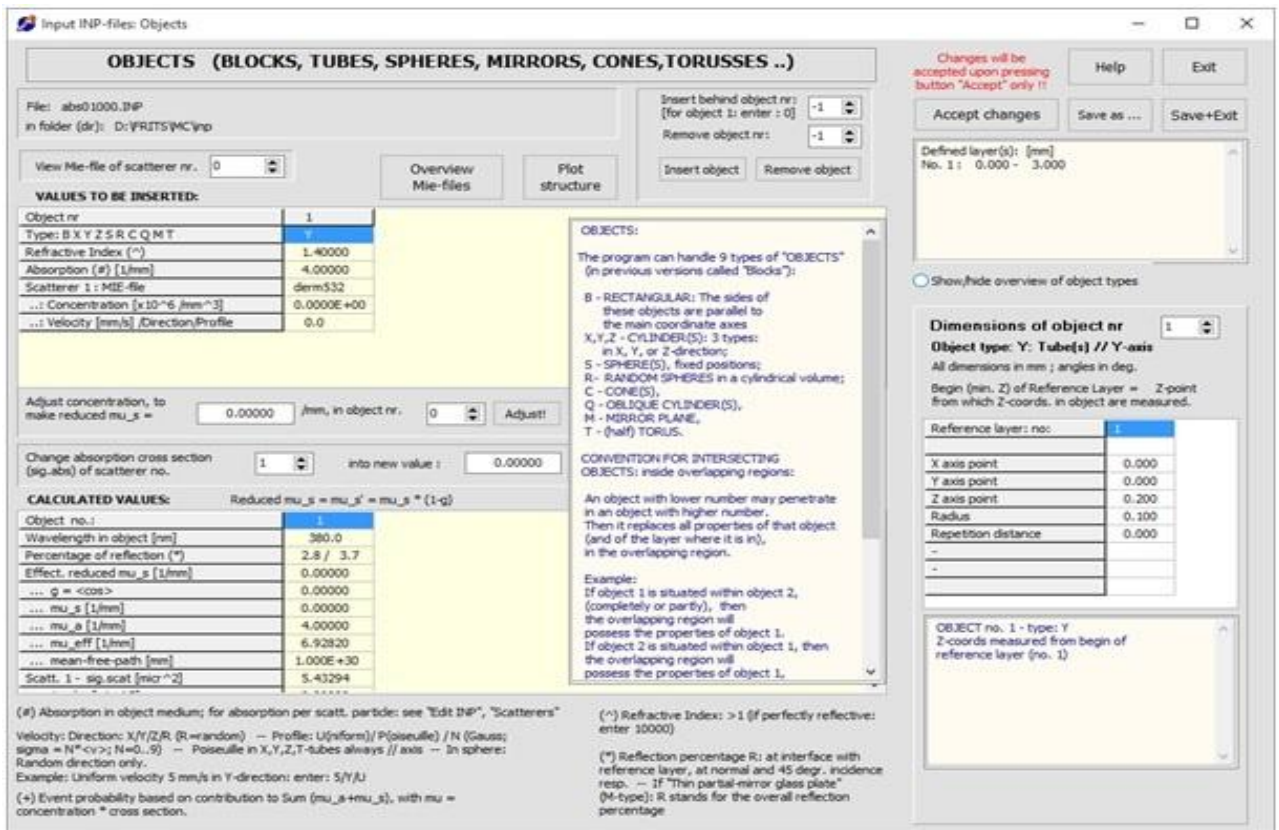


Fig. 19. Input of data for objects (spheres, tubes, mirrors, cones, blocks...)

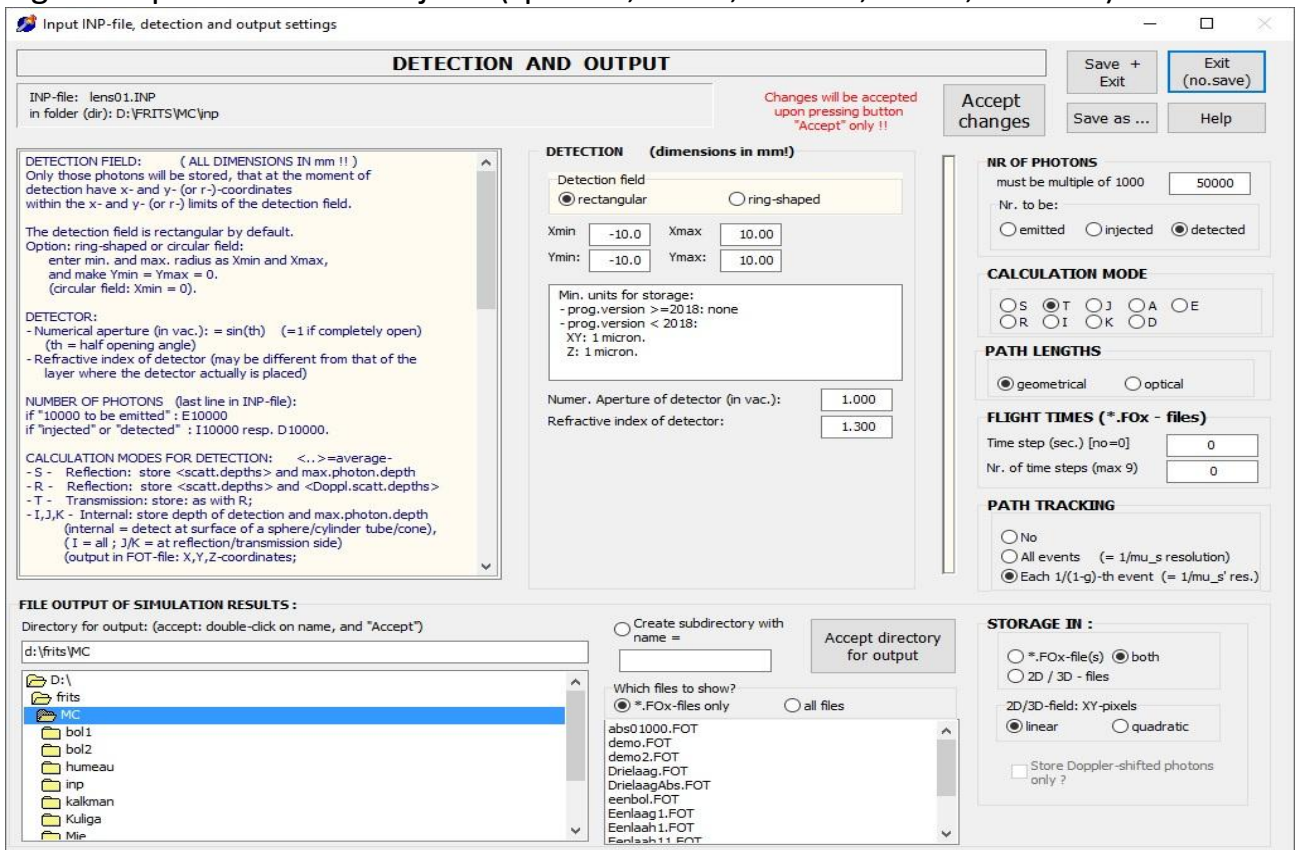


Fig. 20. Detection, calculation mode, flight and path tracking and output

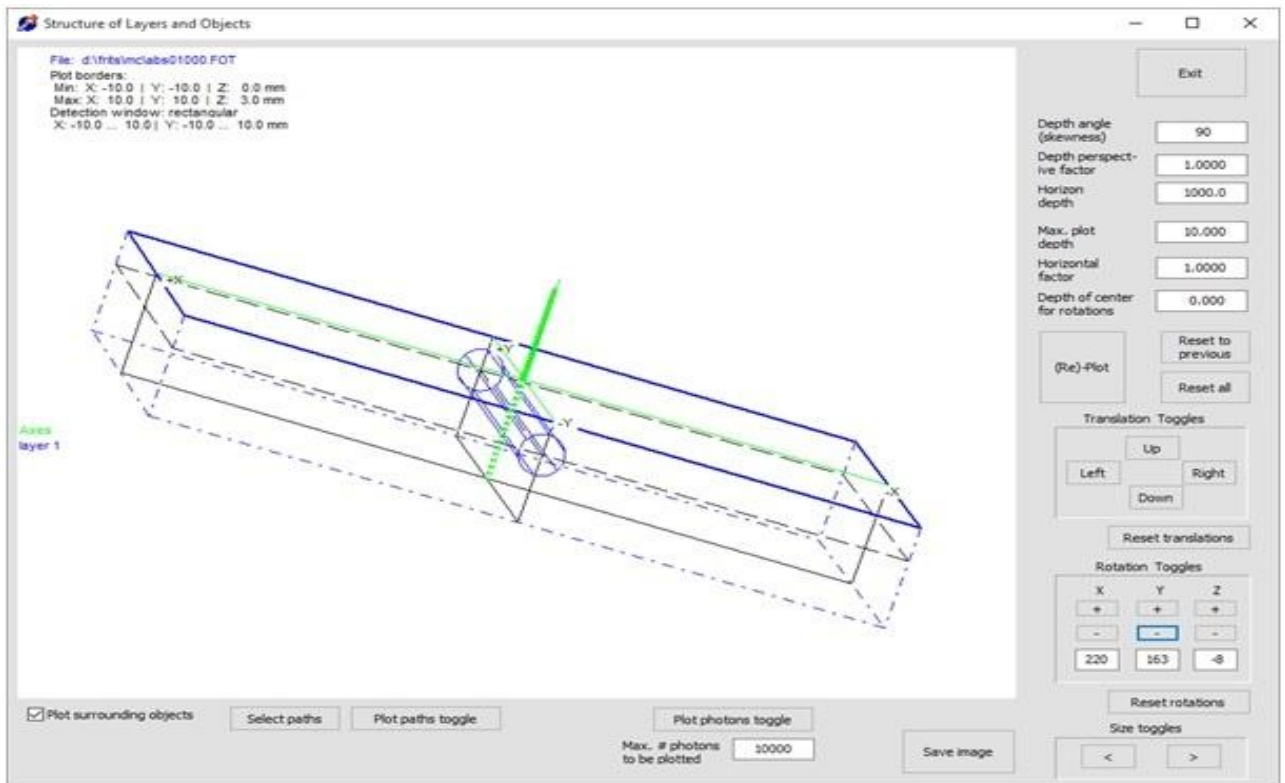


Fig. 11. Structure of the layer system with 1 layer and 1 tube in Y-direction

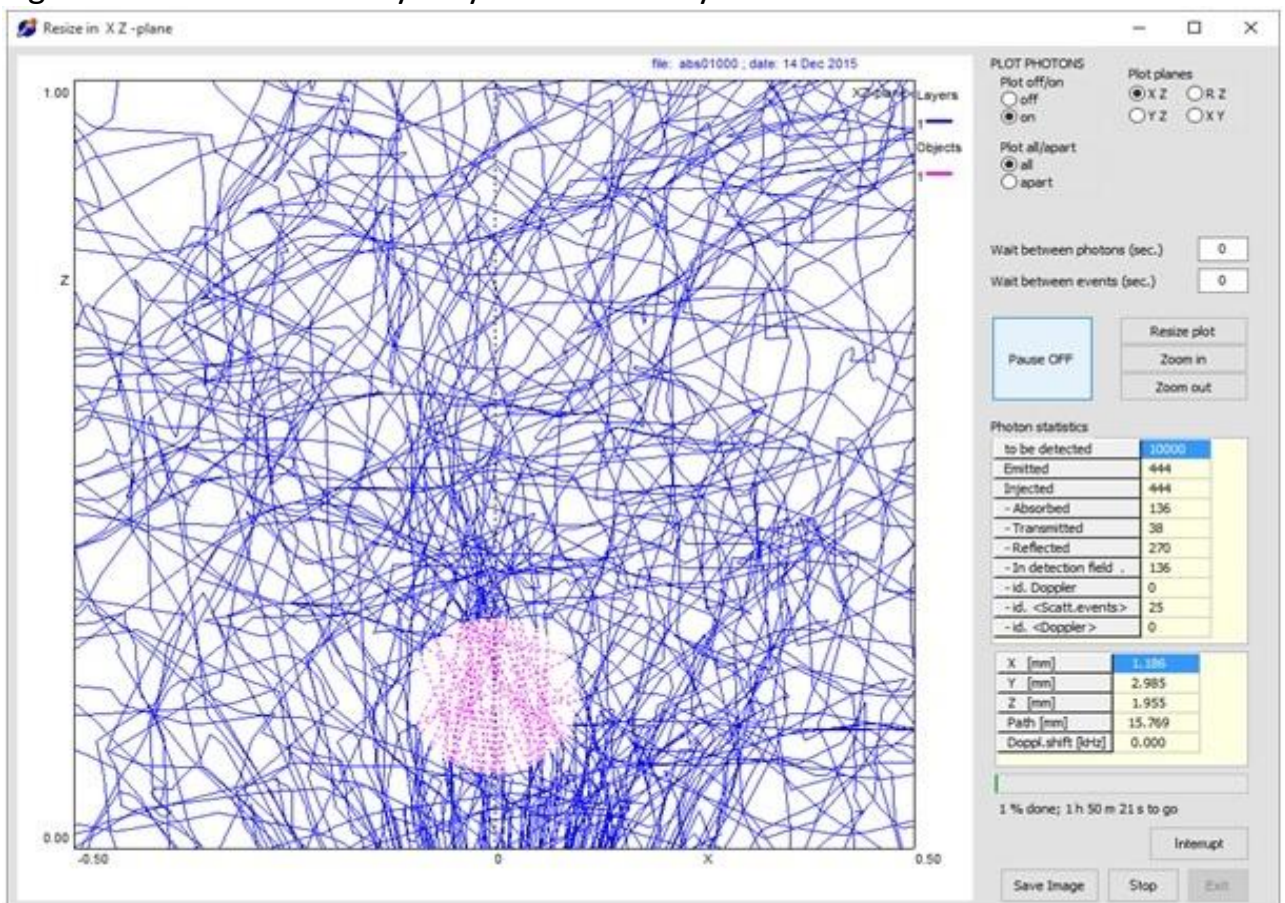


Fig. 22. Simulation of the structure of Fig. 21. View // Y-axis (XZ-plane)

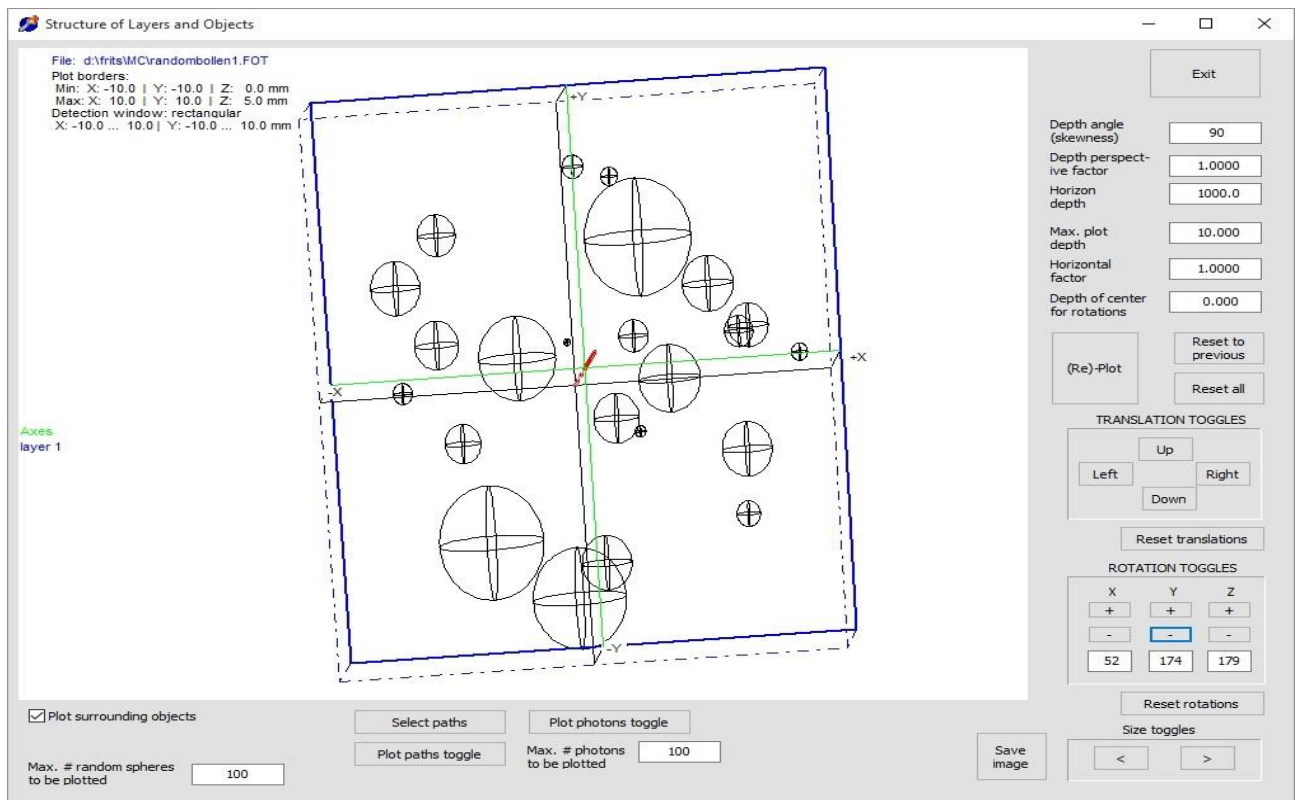


Fig. 23. Structure of a single layer with random spheres

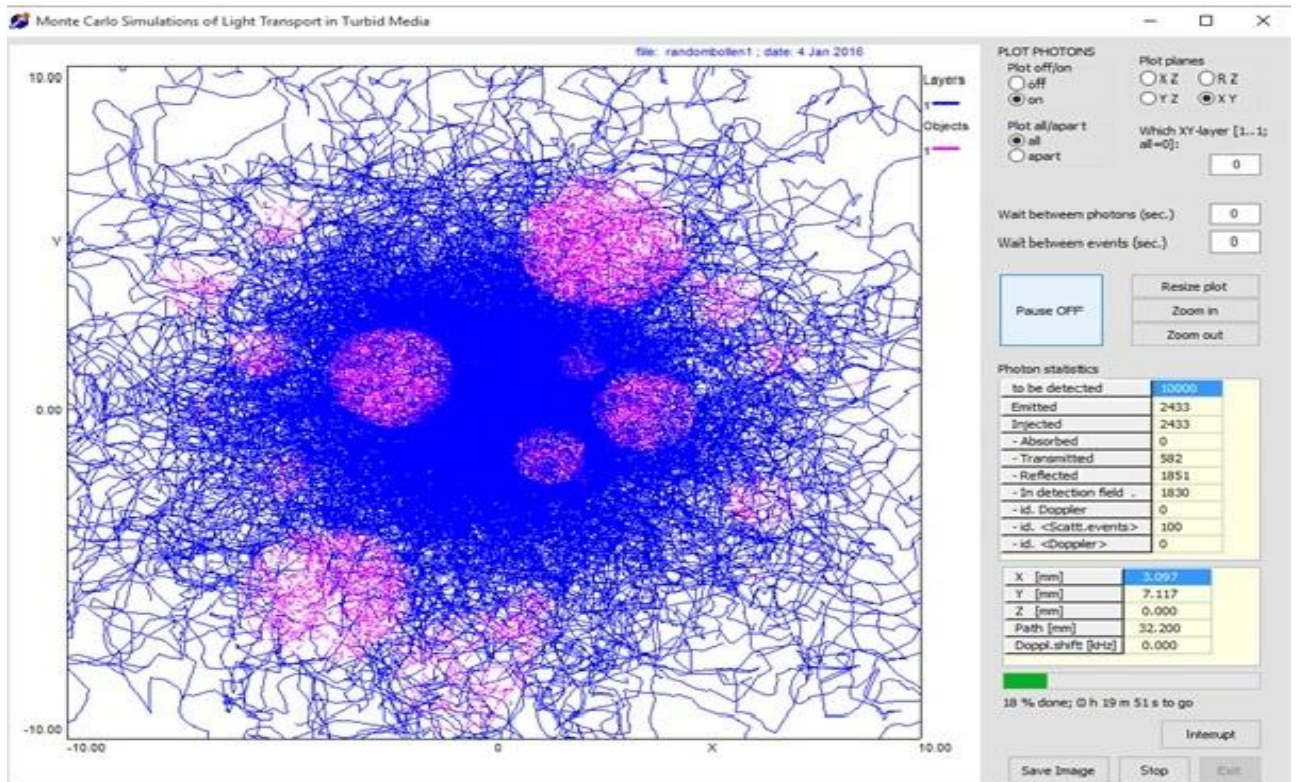


Fig.24. Simulation of the structure of Fig. 23. View // Z-axis (XY-plane)

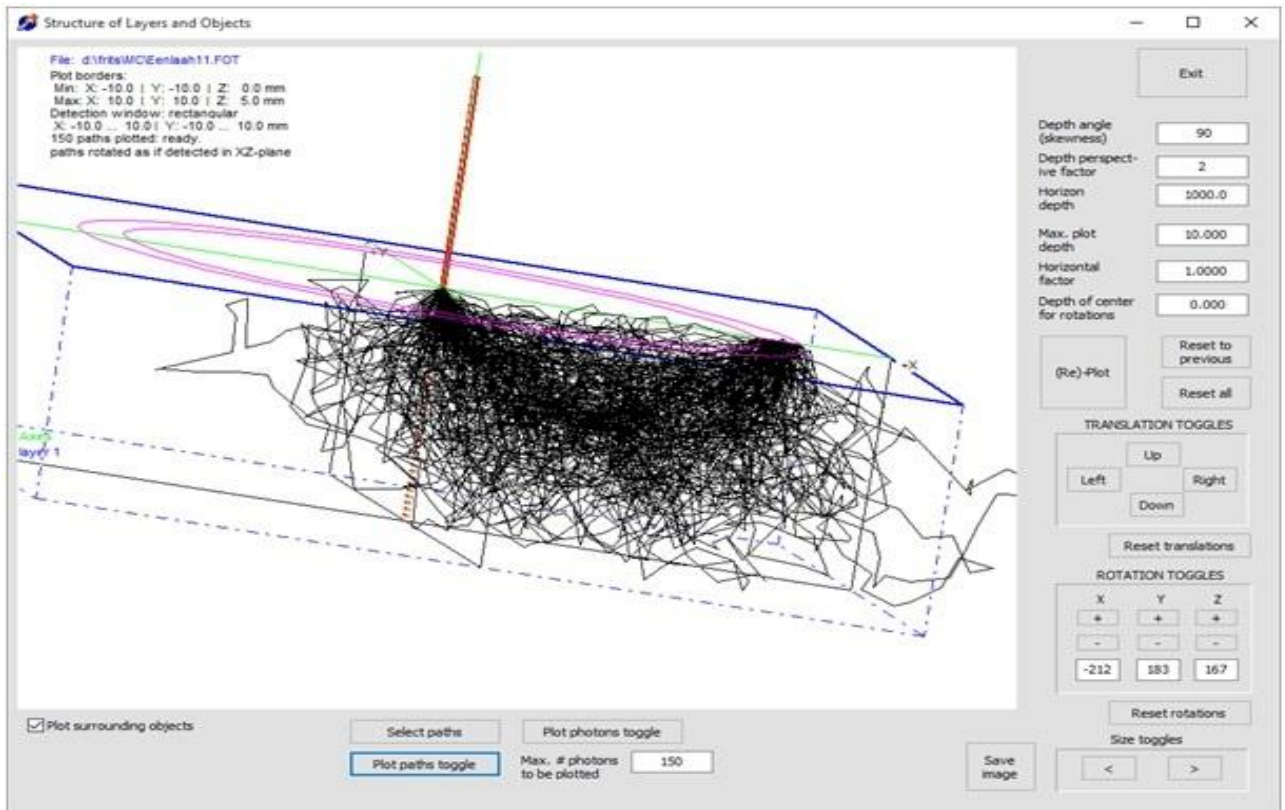


Fig. 25. Path tracking for selected points of emergence. Single layer

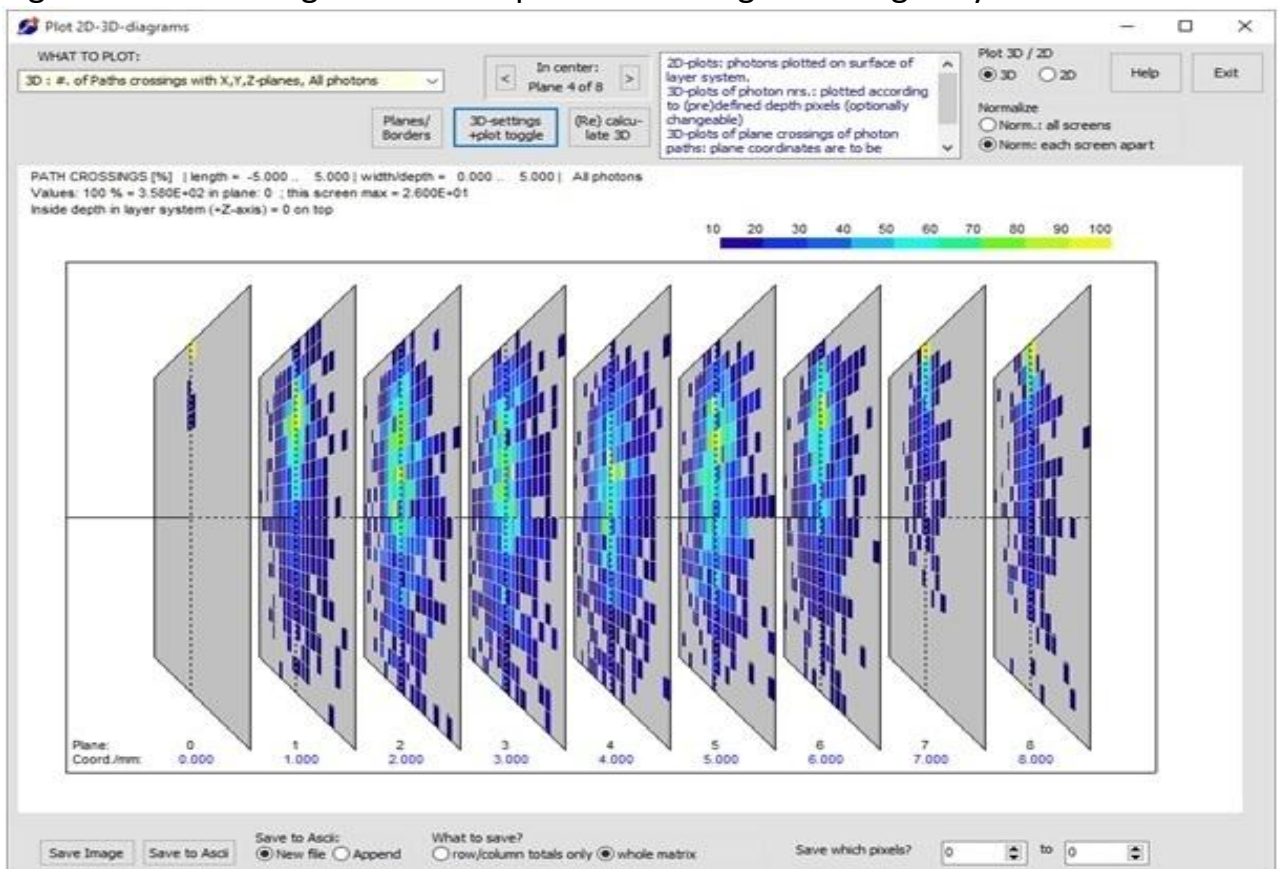


Fig. 16. Path tracking of Fig. 15: crossings with predefined planes; 1 layer.

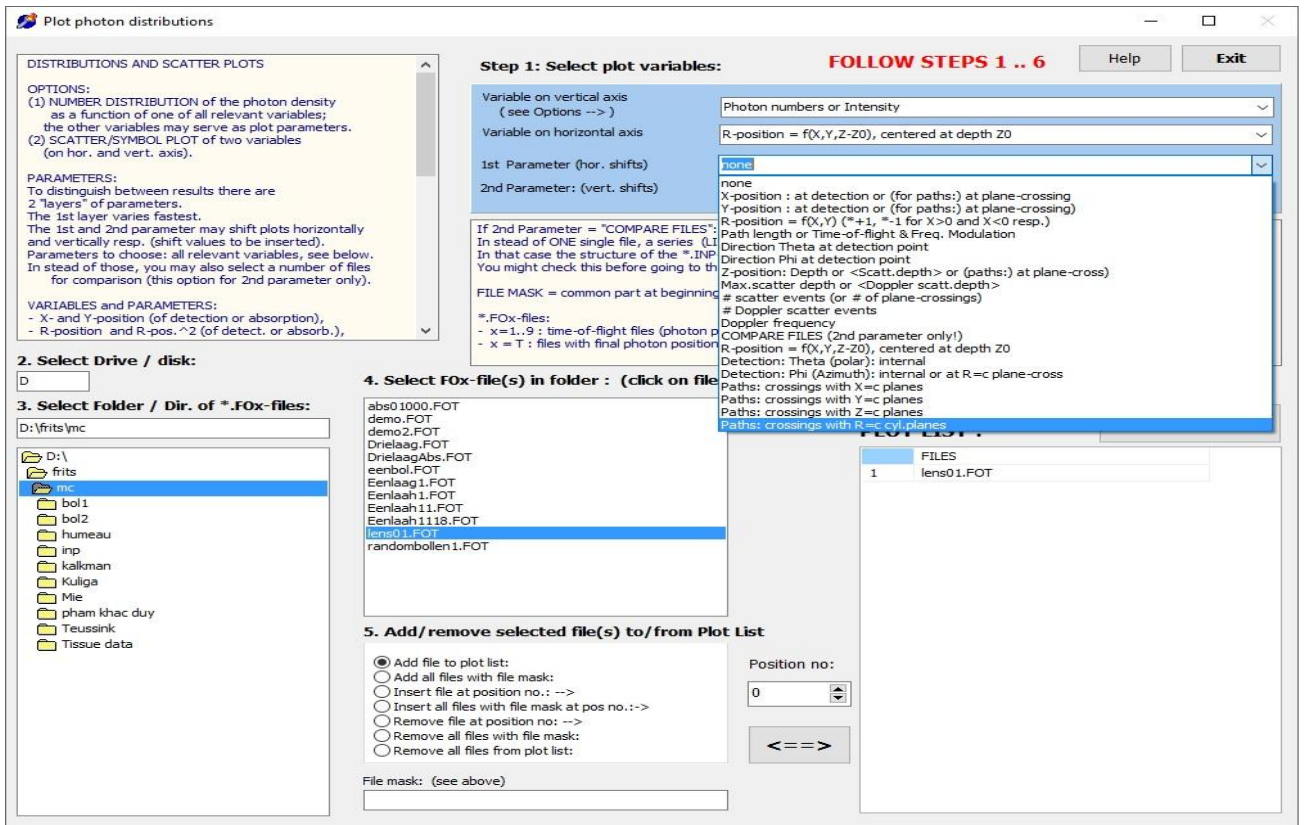


Fig.27. Plot options: choice of axes (“intensity” if vert.axis = none)

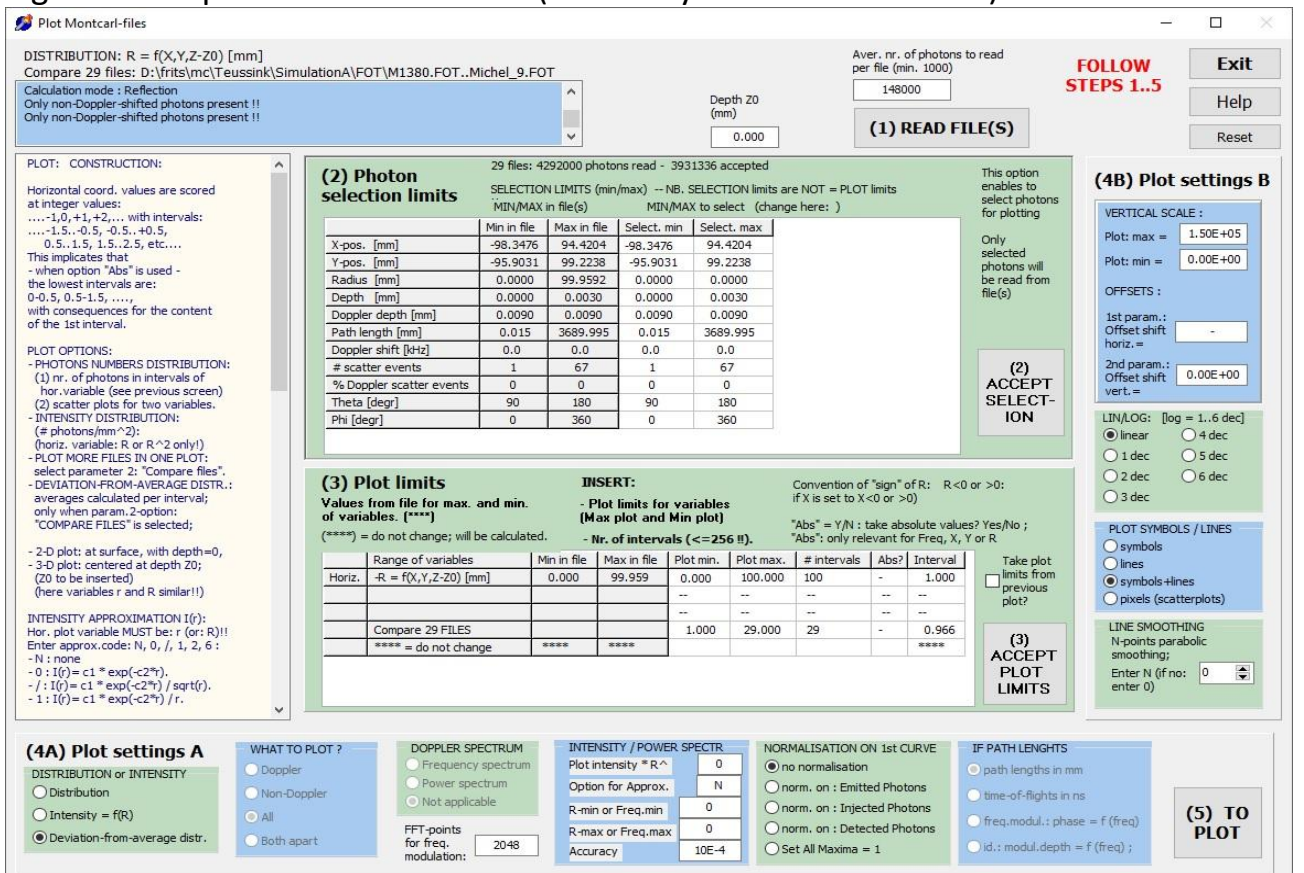


Fig.28. Plot options: settings for an intensity plot

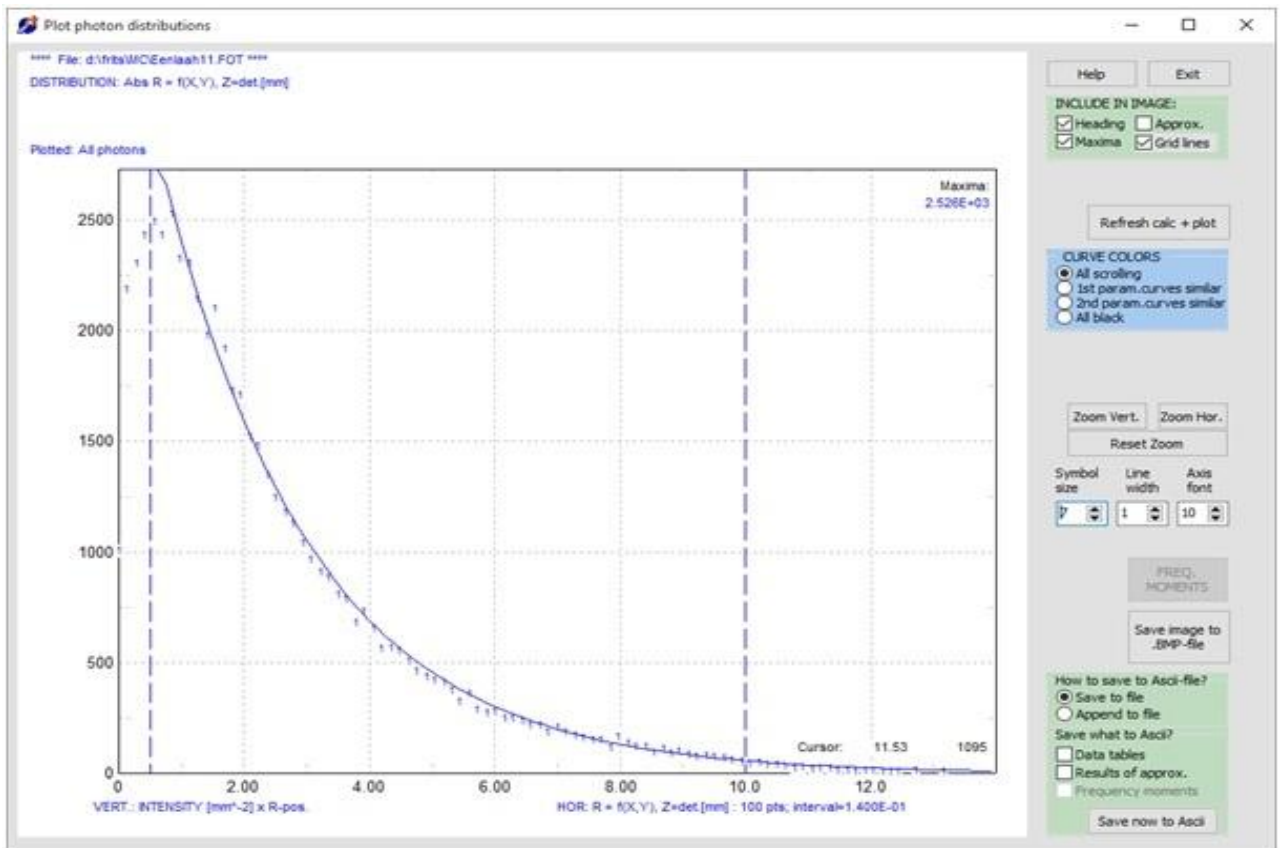


Fig. 29. Intensity plot, with model fitting. Plots of >1 runs optional (with shifts).

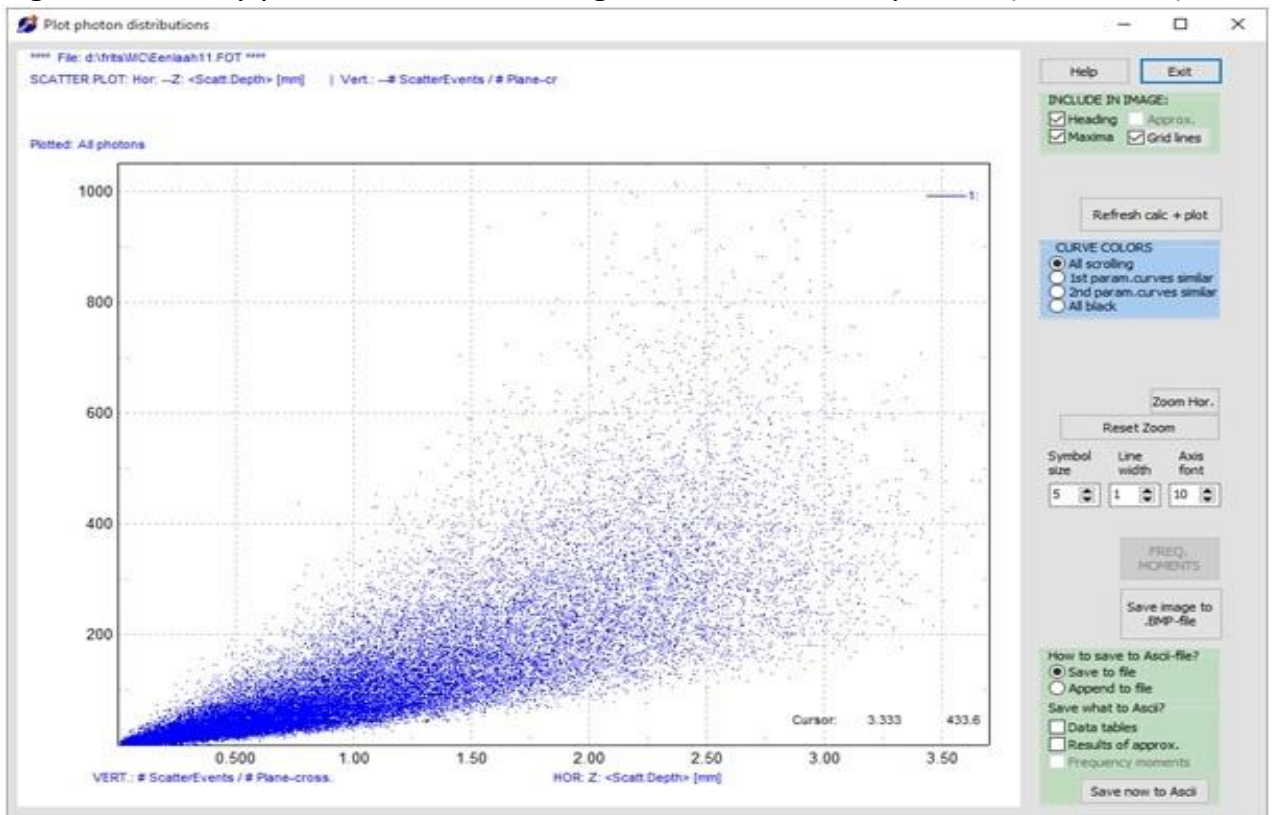


Fig. 30. Scatter plot of results. Plots of >1 runs optional (with vert./hor. shifts)

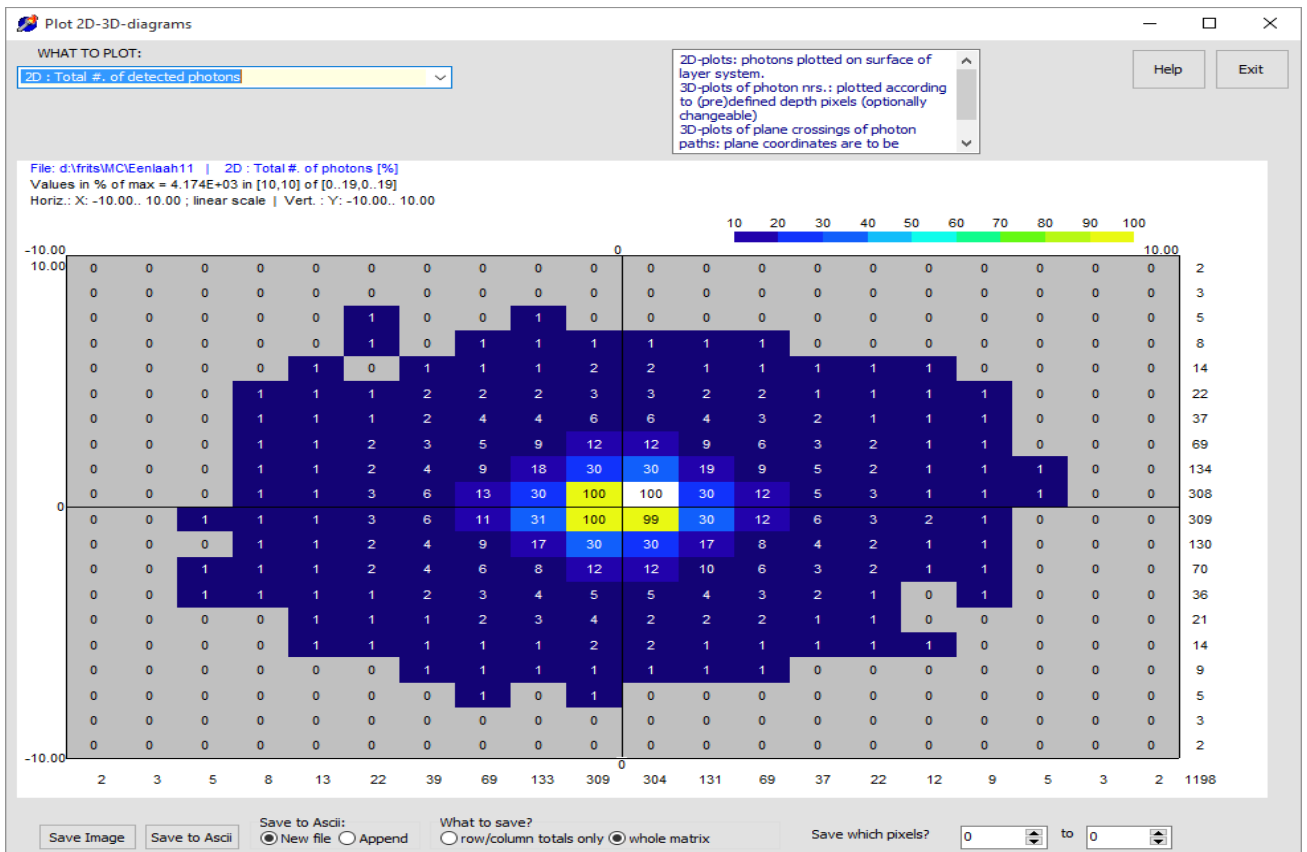


Fig. 31. 2D-plot of results: total number of re-emerging photons.

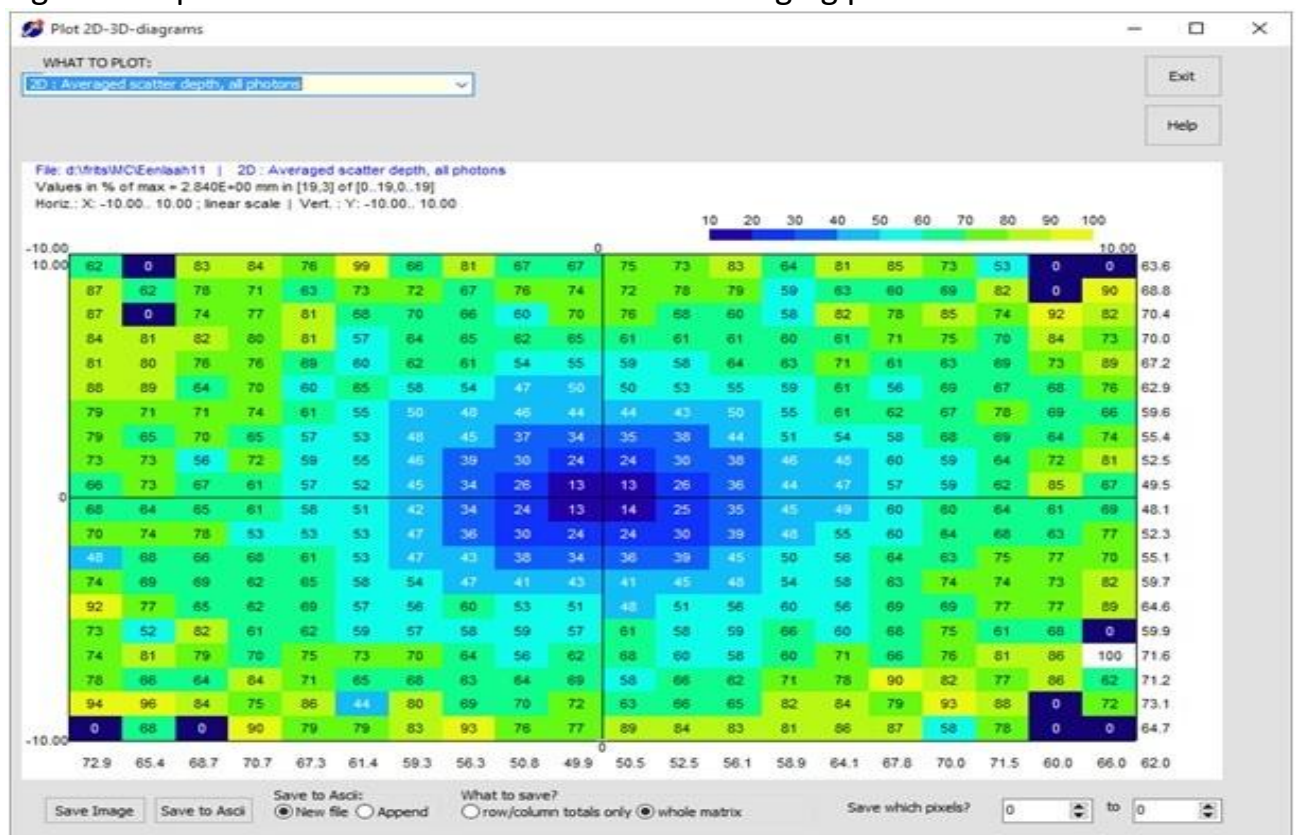


Fig.32. 2D-plot of results: average scattering depth of all photons.

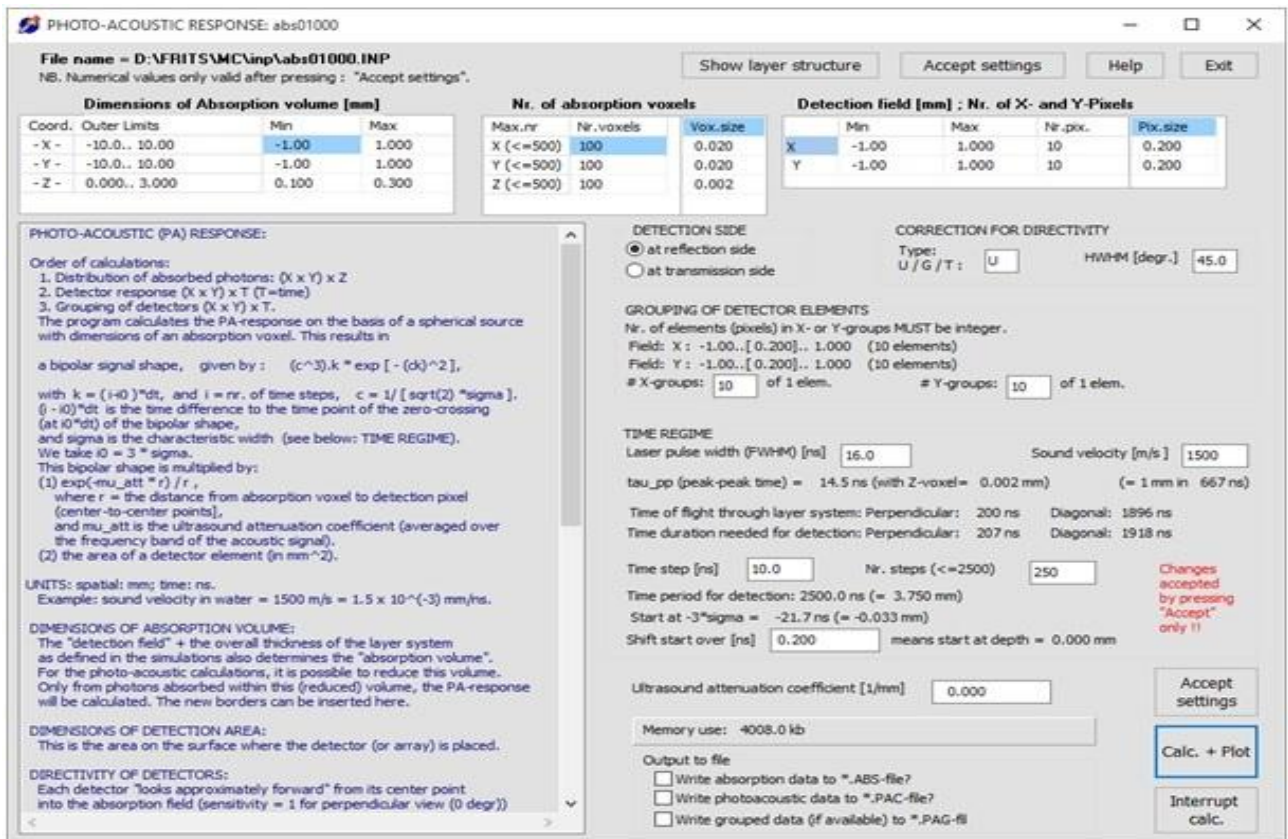


Fig. 33. Photo-acoustic response of absorbed photons: settings

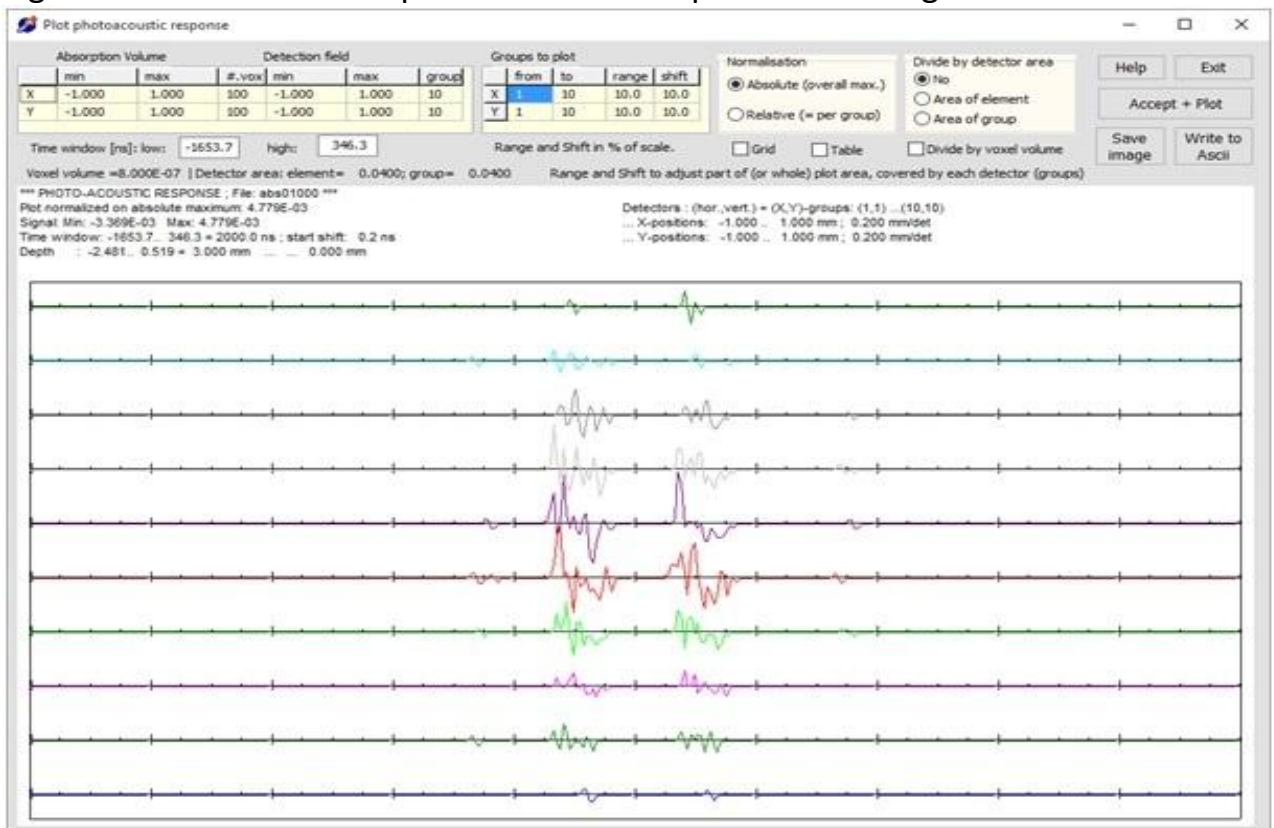


Fig. 34. Photo-acoustic response in 10x10-detector array of 1 tube (Fig.21)

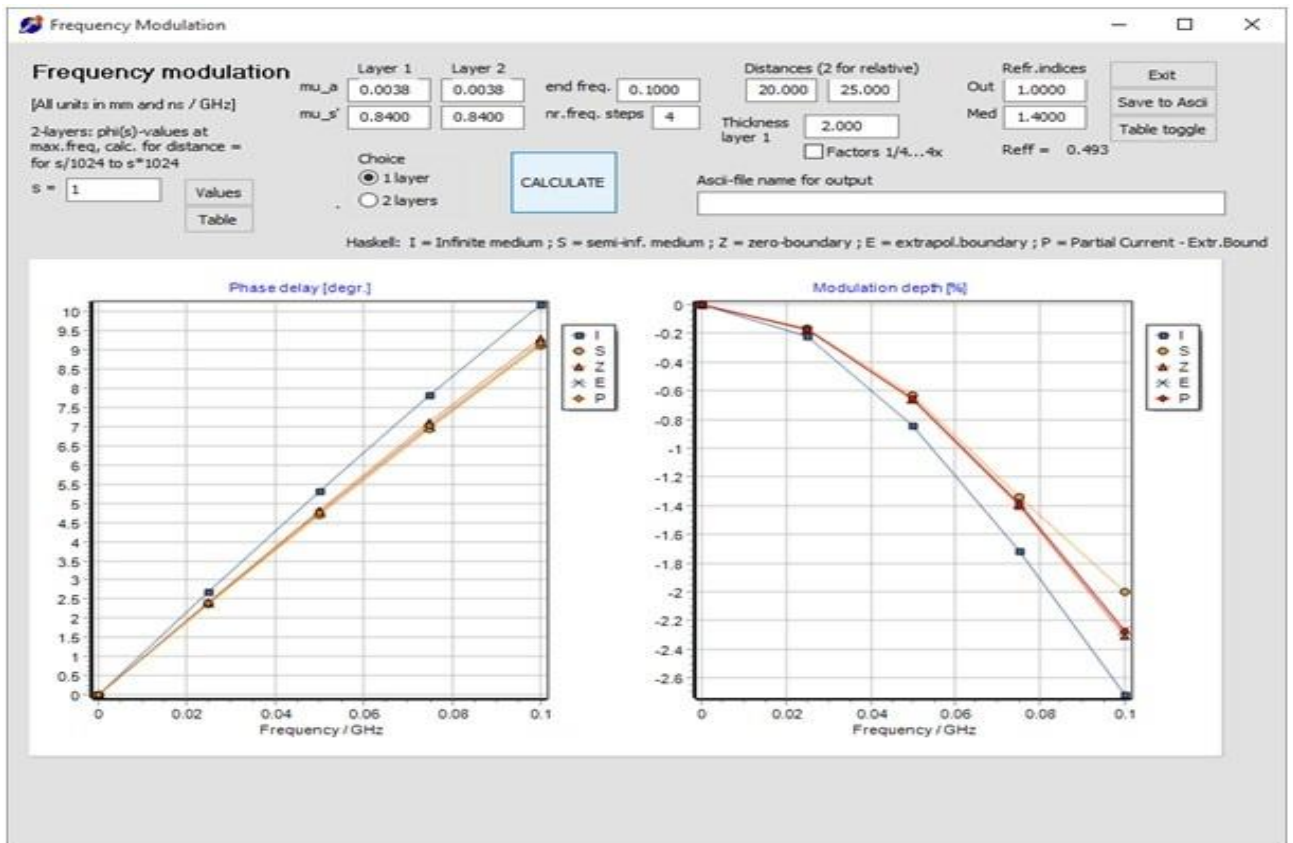


Fig.35. Extra: frequency modulation of GHz-signals in tissue layers.

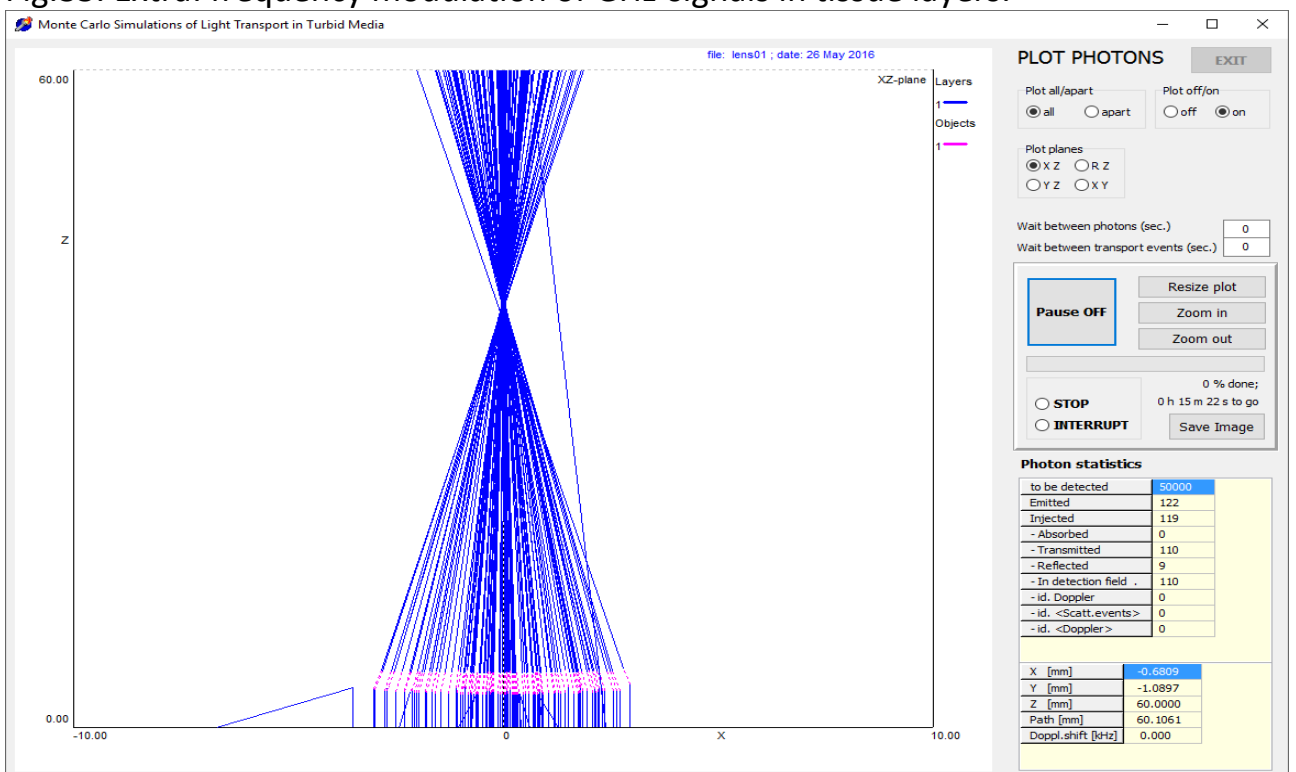


Fig.36. Imaging through a thick convex-concave lens with a few scatterers