Manual for simulation of X-ray processing

Software ModeStXR

Modeling of 3D X-ray dose distribution with MC method. Software ModeStXR.

The program ModeStXR consideration

The **program ModeStXR** was designed specially for simulation of industrial radiation processes and calculation of the absorbed dose distribution within products irradiated by **stationary or scanned X-ray (bremsstrahlung) beams** on industrial radiation-technological lines (**RTL**) that is based on the pulsed or continuous type of electron accelerators in the **energy range** from **0.1** to **50 MeV**. Irradiated product is represented in form of stack of plates. The stack of plates can be interleaved with dosimetric films.

Developed software can be used for the following problem tasks in radiation processing:

1. Determination of dependence of an absorbed dose distribution in a layer as function of:

- X-ray energy spectrum of X-ray converter;
- density and a chemical composition of layer material;
- width and thickness of a layer;
- geometrical arrangement of a layer in a stack;
- density and a chemical composition of a stack layer materials;
- geometrical sizes of a stack;
- an orientation angle of a stack relatively to incident electron beam.

2. Examination of dependence of an absorbed dose distribution in a layer as function of:

- energy of incident EB;
- an EB current and speed of a conveyer motion;
- an angular distribution of electrons in a beam;
- a spatial distribution of electrons in a beam;
- a width of EB scanning;
- an angular characteristics of a scan process;
- a time sweep of the scanner;
- an air gap between the scanner and X-ray converter and an irradiated target target.

3. The comparative analysis of visual and numerical difference of depth-dose distributions in a layer for:

- various parameters of calculation;
- various calculation models;
- an experimental and calculated depth-dose distributions in a layer.

The features of the software **ModeStXR** are as follows:

- 1. Two levels for entering of input data via configuration files and manually.
- 2. Built-in tools for statistical analysis.
- 3. Built-in tools for uncertainties estimation of results simulation due to uncertainties of input data for radiation facility.
- 4. Estimation of uncertainties for physical models.

5. Comparison Modulus for visual and a numerical analysis of calculated and experimental data and

for decision of optimization tasks in radiation processing.

6. Built-in tools for processing of experimental dosimetric data and their comparison with simulation predictions.

The software have intuitively clear graphical interface for the end-users with the following features:

1. Detailed decomposition of input data for main elements of source and target (including spectral characteristics for irradiation source).

2. Two levels for entering of input data via configuration files and manually.

3. Expert control for the range of input data and co-ordination for the set of geometrical and physical input data.

4. Compatibility of export an input data to different modules.

The software **ModeStXR** works on platform Windows98/Me/NT/XP/2000. Language of the interface - English.

Software ModeStXR. How to get results.

🚖 ModeStxr 3.1 (2008) 💶 🗖 🗙	
<u>File Options H</u> elp <u>A</u> bout	For work with software ModeStXR -
Number of	• Click the "File" then "Open
10000	configuration", then to select "irradiating
	system" and load the file "Test.rts".
	• Again click the "File" then "Open
Converter	configuration", then to select, "irradiated
	target and load the life lest.rtt.
	• Again click the "File" then "Open
Target	and load the file "Test rte"
	and load the me rest.it.
Simulation	Only after loading the "Test.rts", "Test.rtt"
	and "Test.rtc" files, user can change all
Stop	characteristics of X-ray facility and irradiated
10:05:14	target for simulation X-ray processing.
	If all input data are saved, color of the
	scheme item changes to blue.
	• Enter "Number of trajektories" and
View results after simulation	• Chiele the hetter "Simulation"
Open and view results from file	• Click the Dutton "Simulation".
Comparison	At this point the software modestax fixes starting time and defines time required for
	calculation.
Click Source,Scan,Target,Converter	• Click "Stop" to interrupt your calculation
Fig 1 The main form of the	and reenter data.
Software ModeStXR	• When MC will be ended, the list of results
	will be opened.
	You can select item and work with results.

Input data

1. Source



• Click "Source" in the Scheme of Monte Carlo Module, MC. See Fig. 2.

The form for Source – Electron Accelerator parameters will be opened. See Fig. 3.

Fig.2. Scheme of MC Module

🚧 Source		×
Beam current	Spectrum	Angular spread
✓ Pulsed regime Average current (mA) 1 Impulse current (A) 10 Impulse time (mSec) 2 Repetition (Hz) 50	MonoEnergy Energy (MeV) Image: Spectrum Image: Spectrum N Rows Image: Spectrum Image: Spectrum Image: Spectrum Image: N Rows Image: Spectrum Image: Spectrum Image: Spectrum Image: S	MonoDirect Angular spread N Rows 2 Correct table Angle Insens. 0,000 1,000 6,000 1,000
	Space spread	
☐ Point beam ✔ Distributive beam	Beam diameter (cm)	Full width on half maximum (cm)
	5	Save data and close this window

Fig. 3. The main form of "Source" for data input and correction of an Electron Accelerator parameters.

1.1. Beam current

The frame **Beam current** contains some fields.

There are two regimes for input data: "Pulsed regime" and "Average current".

- Click the "Pulsed regime" by a tick, to work with Pulsed regime data.
- Enter the values Impulse current in A, Impulse time in msec, Repetition frequency in Hz.
- Delete a tick from window "Pulsed regime", to work with "Average current" mode.
- Enter the value of Average current in mA.

1.2. EB energy spectrum

Fields for **EB** energy are placed into the frame Spectrum.

- Click the field "MonoEnergy" with a tick, to work with MonoEnergy mode.
- Enter a value of the Energy.
- Click the field "Spectrum" with a tick, to work with EB energy spectrum mode.
- Enter a rows number in the table, Click button "Correct table".
- Enter or edit table data.

A left mouse button allows to insert a row in the table or delete selected row. When rows number is changed by left mouse button, the field **N** rows will change accordingly. At this point **Energy** field will be inaccessible.

1.3. Angular spread

- Click the field **MonoDirect** by a tick, to work with **MonoDirect** mode. The target will be irradiated with non-divergent scanned electron beam.
- Click the field Angular spread by a tick, to work with Angular spread mode.
- Enter a rows number in the table, Click button "Correct table".
- Enter or edit table data for the beam angle spread.

You work with this table by analogy with the table of EB energy spectrum.

- Enter data of space spread, to work with the frame Space spread.
- Click the field "Point beam" by a tick, to work with Point beam mode.
- Click the field "Distributive beam" by a tick, to work with space spread mode.
- Enter data of Beam diameter in cm and Full width on half maximum in cm.
- Click the button "Save data and close this window".

Image of "Source" in the Scheme of Monte Carlo Module change into blue color.

2. Scanner

• Click "Scan" in the Scheme of Monte Carlo Module. See Fig. 2. The main form for Scanner and Conveyer parameters will be opened. See Fig. 4.

• Enter values of Speed in cm/sec and Width in cm in the frame Conveyer.

• Enter values of Frequency in Hz and Height of scan horn in cm in the frame Scanning horn.

葦 Scanning system (Mi	odeStxr 3.1 2008)	×
	Scanning system	m
Conveyor	Scanning horn	₩ Window of scaner
Speed [cm/sec]	Frequency [Hz]	Thickness [cm]
1	10	0,005
Width [cm]	Height [cm]	Density [g/cm3]
100	100	4,5
Geom	etry	Regimes of scanning
Scan-conv. distance [cm]	Scanning width [cm]	 □ Non-diverging beam □ Default mode ✓ Triangular scanning ✓ Custom mode
65	60	N Rows 5 Correct table
		Time Current
		2 0,24
		Save data and close this window

Fig.4. The main form for the Scanner and Conveyer parameters.

• Enter values of Distance scan-conveyor in cm and Width of scanning in cm in the frame Geometry.

• If you have linear time-current curve in scan magnet (saw-tooth form of current), you need to mark the check box of "Default mode" by a tick.

• Mark the check box of "Custom mode" by a tick, if you have nonlinear timecurrent curve.

• Enter a rows number of the table, press button "Correct table" and work as well as with tables for an electrons source. The values of time and current are dimensionless.

• You can Enter the foil parameters of the outlet window of scanner.

For this, you need to mark the frame "Window of scanner" by a tick. The frames for the foil parameters will be opened.

- Enter values of Thickness in cm, Density of foil material in g/cm³.
- Enter values of "Atomic number" and "Weight part" for the foil material.
- Click the button "Save data and close this window". Image of "Scan" in the Scheme of MC Module change into blue color.

3. Converter

• Click "Converter" in the Scheme of Monte Carlo Module. The main form for Converter parameters will be opened. See Fig.5.

茸 Input data for	a Brem	sstrahlı	ung radi	ation (H	dodeSt	xr 3.1 20	08)			
[)istance	between	converter	r and sca	an 1					
Elements	Layer 1		Layer 2		Layer 3		Layer 4		Layer 5	
Thickness [cm]		0,12		0,5		0,2				
Density [g/cm3]		16,6		1		7,9				
Material	Z	W	Z	W	Z	W	Z	W	Z	W
	73	1	1	2	26	1				
laver			8	16						
2										
Clear layer										
						Save c	lata and o	close th	iis window	/

Fig.5. The main form for data input and correction of the **Converter** parameters.

X-ray converter has multi-layer structure. The numbers of flat layers are in the range from 1 to 5.

The functions of layers are as follows:

- X-ray converter plate,
- cooling agent and
- backing plate for absorbing of electron beam.
- Click on layer 1 or 2 or 3 or 4 or 5.

In this point the column of corresponding layer will be activated and in the Layer field will be shown the layer number that will be corrected. Instead you can type the layer number in Layer field.

- Enter for this layer material: Thickness layer, Density, atomic number Z , and W ("weight part").
- Enter Z and W for each element of compound and mixtures .
- Enter values of Distance between converter and scan in cm.
- For clear data in selected layer, enter layer number in the Layer field and click the Clear layer

• Click the button "Save data and close this window". Image of "Converter" in the Scheme of MC Module change into blue color.

4. <u>Target</u>

4.1. The form for entering of input data for irradiated Target and Cover

• Click "Target" in the Main form of the Software ModeSXR (See Fig.2).

The form for entering of input data for irradiated Target and Packing materials (Cover) will be opened (See Fig.6).

韋 Target and cov	er	(ModeStxr 3.1 200)8)													×
Number of package	s	Multi - Target Distance between targets	0,01	_	0	rientat ● Ver	i <u>on</u> tical	0	Along Along	the so the co	cannin onveyo	g axis raxis		⊙ N O Tu	ormal displa um on 90 de	cement g
Width of packages	t	Current layer	6				Delete			Insert			Clear			
40,01	r r	Layer	11		2		3		4	ļ	5		6)	J	
Ohe als law with	a l	Thickness	5		2		0,5		5		8		5			
Stack length	e	Width	40		40		40 7 9		40		40		40			
20	t	Polyethylene	Z	Ιw	Z.	l w	Iz	lw	Z	1 w	l z	l w	4 Z	1 w		
2D registration		Poliystyrene	1	2	13	1	26	1	1	2	1	10	1	8		
package + layer		PMMA Carbon	8	16					8	16	6	72	6	60		
PL		Birchwood									8	80	8	32		
1 1		Soft Tissue														
1 2		Water 🛄														
1 4																
1 5	_	Danaitu	1			Γ	Polivets	rono			N	List			Opened c	over
Ь	ŏ	Density	<u>P</u>			F	PMMA	riciic				Tabl	е			
	v	Cover thickness	0.5				Carbon Birchwo	bod								
IM 3D calculation	e	Cover Inickness	10,0			(Cellulos	se			3		An	umbarl	Ul nort	-
<u>3D registration</u>	r	Additional cover	0				Vater	sue			Ro	WS	1	unber	10	
package + level							eflon Numini	Im					6		72	
						i	ron						8	1	30	
						ļ,	Anothe	r mate	rial	•			,			
					21										1	
Thickness, width,	ad	ditional cover [cm]; D	ensity	([g/cm	3]					5	ave da	ata and	d close	e this w	indow	

Fig.6. The form for entering of input data for an irradiated Target and Packing materials (Cover).

4.2. Multi-layer target model

• Multi-layer target consists of some identical packages with flat sheets of materials with various density and atomic number. (See Figs.7 and 8).

Geometrical models of multi-layer targets irradiated with scanned X-ray beam.





Conveyer moves along axis Y. X-ray beam scans along axis Z.

- a) Multi-layer target consists of 6-layer package placed in closed packing box with additional packing materials.
- b) Multi-layer target consists of two 6-layer packages placed in open packing box.

• The number of packages are in the range from 1 to 10.

• The number of layers (flat sheets of materials with various density and atomic number) in the each package are in the range from 1 to 6. (See Figs.7 and 8)

- The full number of layers in Multi-layer target are in the range from 1 to 60.
- All packages have the same set of materials and identical geometrical sizes.

• All flat sheets of 6 layers in the package can have different thickness (axis Z) and width (axis X, along scan direction), but all sheets have identical length (axis Y, along conveyer motion).

• Multi-layer target can be located on the conveyer platform with/without packing box.

• Several identical Multi-layer targets with/without packing box can be located on the conveyer platform. (See Fig. 9).

The distance between boxes with Multi-layer targets can be ≥ 0 .



Fig. 8. Geometrical models of multi-layer targets irradiated by incident

X-ray beam in parallel with interface of contacting materials. Conveyer moves along axis X. X-ray beam scans along axis Z.

- (a) Multi-layer target consists of two identical 6-layer packages placed in open packing box and irradiated by incident X-ray beam in parallel with interface of contacting materials.
- (b)Multi-layer target with dosimetric films inserted between interface of contacting materials and irradiated in parallel with X-ray beam.

Simulation of the dose distribution in the "Several identical Multi-layer targets with/without packing box" allows to investigate the mutual influence of the nearest neighbor boxes on dose field formation in the target layers.

• The flat sheets of Multi-layer target can be located on the conveyer platform horizontal or vertical relatively incident X-ray axis. (See Figs. 7 and 8).

<u>Note.</u> In any layer positions under X-ray irradiation, axis coordinates X, Y, and Z are hard connected with width (X), length (Y), and thickness (Z) of target layers (See Figs. 7 and 8).



D- distance between boxes

Fig. 9. Geometrical model of 3 identical Multi-layer targets with packing box located on the conveyer platform. The distance between boxes with Multi-layer targets can be ≥ 0 .

4.3. Input data for layers size and layers materials

• Enter the number of packages in multi-layer target in the range from 1 to 10.

• Enter the number of layers in the package in the range from 1 to 6.

For this, Click the button "Insert" (right up corner in the "Target" frame) (See Fig. 6).

• Enter the "Width of packages" in cm (left up corner in the "Target" frame) (See Fig. 6).

- Enter for each layer "Thickness" in cm.
- Enter for each layer "Width" in cm.

<u>Note.</u> The "Width of packages" can be \geq "Width" of each layer.

• Enter for each layer "Density of materials" in g/cm³.

• Select a material for each layer from the "Table of material". The atomic number

Z and the **atomic weight W** of the material appear in the corresponding boxes.

• For materials not given in the **"Table of material"**, enter the values of **Z** and **W**. The selection button changes to **"Another material"**.

- Button "Delete" is used for deletion of the chosen layer.
- Button "Clear" is used for cleaning of the parameters in the chosen layer.

4.4. Input data for cover size and cover materials

- Enter characteristics for the "Cover Box": "Cover thickness" in cm, "Additional cover thickness" in cm, and "Density of cover materials" in g/cm³. Note. In the case of cover thickness = 0, the multilayer target has not a Cover Box.
- Select a material for cover materials from the "Table of material".

The **atomic number Z** and the **atomic weight W** of the material appear in the corresponding boxes.

• Enter the values of Z and W for materials not given. The selection button changes to "Another material".

• Multilayer target can be irradiated by incident X-ray beam either in closed or open (Tick window "Opened cover") Cover Box. (See Fig. 6).

4.5. <u>Input data for layers orientation on a conveyer platform under</u> <u>X-ray irradiation</u>

• Simulation model of the software ModeSXR for target irradiation allows to irradiate the box with flat layers from any of six box sides. Selection of target orientation relatively incident X-ray beam is realized with the switch "Orientation" (See Figs. 6 and 10).



Fig. 10. Frame with mode switch of orientation for target layers under X-ray beam irradiation

• Switch positions ("Vertical" and "Normal displacement") in Fig.6 are used as default mode. This target position is mean that all flat target layers are located on conveyer platform in accordance with position in Fig.11.1.

I.e. the planes of all layers are perpendicular to axis of incident X-ray beam. The **length** of layers is located in direction of conveyer motion (axis Y), the width – in direction of X-ray beam scanning (axis Y), the thickness – in direction of X-ray beam incidence (axis Z). (in parallel with an incident X-ray beam (axis Z))

• All possible positions of layers orientation on a conveyer platform under X-ray beam irradiation and corresponding switch positions are presented in Figs. 11.1, 11.2, 11.3, 11.4, 11.5, 11.6.

• <u>Note.</u> In any layer positions under X-ray beam irradiation, axis coordinates X, Y, and Z are hard connected with width (X), length (Y), and thickness (Z) of target layers.

• All above possible positions under X-ray beam irradiation also can be realized for package of flat layers placed in open/closed box (See Figs. 12.1 and 12.2) and for package of flat layers placed in open/closed box with additional cover (See Figs. 13.1 and 13.2). Additional cover always covers only the box sides in direction of layers thickness (along axis Z).



Fig.11.1

Fig. 11.2





Fig. 11.4













Fig. 12.2

Figs. 12.1 and 12.2. Some possible orientation positions on a conveyer platform for package of flat layers placed in open packing box



Figs. 13.1 and 13.2. Some possible orientation positions on a conveyer platform for package of flat layers placed in open packing box with additional cover and corresponding switch positions

4.6. <u>Input data for irradiation of some identical Multi-layer targets</u> <u>with/without packing box</u>

Simulation of the dose distribution in the "Several identical Multi-layer targets with/without packing box" allows to investigate the mutual influence of the nearest neighbor boxes on an X-ray dose field formation in the target layers.

- Tick the window "Multi-target". (See Figs. 2, 6 and 14).
- Enter the value "Distance between targets" in cm.

The distance between boxes with Multi-layer targets can be ≥ 0 .

Multi - Target	
Distance between targets	5

Fig.14. The form for entering of input data for Multi-target.

4.7. Input data for Table "2D registration"

The Table "<u>2D registration</u>" allows to chose the **number of packages** and the **number of layers** for which the results of simulation for absorbed dose distribution (ADD) will be presented in the 2D graphical and tabular forms. (See Figs. 6 and 15).

<u>2D req</u> packa	gistration Ige + level
Р	L
1	1
1	3
2	1
2	3
3	1
3	3
I I▼ 3D	calculation
<u>3D re</u>	gistration
packa	ige + level
<u>Р</u> 1	L 3

Fig.15. The form for entering of input data for Table "2D registration and 3D registration".

• Select in the Table "2D Registration" the number of packages and

the **number of layers** in chosen package for which the results of simulation for absorbed dose distribution (ADD) will be presented in graphical and tabular forms.

• Note. The Table "2D Registration" includes the number of packages "P" and the number of layers "L" in chosen package "P".

• For one run simulation the number of packages "P" can be chosen in the range from 1 to 6 of 10 packages, and the number of layers in chosen package "L" can be chosen in the range from 1 to 6.

• For obtaining of the values for **ADD** in another packages and layers, you need to enter the number of appropriate packages and layers in the **Table ''2D Registration''** and repeat the run simulation.

In this way, you can obtain step by step the **ADD** in all layers of multilayer target.

4.8. Input data for Table "3D registration"

The Table "<u>3D</u> registration" allows to chose the number of one of packages and the number of one of layers in the chosen package for which the results of simulation for analysis of the 3D absorbed dose distribution (ADD) of X-ray beam will be presented in the graphical and tabular forms. (See Figs. 6 and 15).

• Tick the window "<u>3D calculation</u>". (See Figs. 6 and 15).

• Select in the Table "<u>3D registration</u>" the number of package P and the number of layer L in the chosen package P, for which the results of simulation will be available for analysis of **3D** absorbed dose distribution (ADD) in graphical and tabular forms.

• For obtaining of the values for **3D ADD** in another packages and layers, you need to enter the number of appropriate package and layer in the **Table** "**3D registration** " and repeat the run simulation.

In this way, you can made analysis of the **3D ADD** of **X-ray beam** step by step in all layers of multilayer target.

At the end, Click "Save data and close this windows".

The selected parameters for multilayer target will be saved and ready for simulation.

5. Options

Options are intended for:

- optimization of simulation regimes,
- optimization of parameters visualization of calculated results,
- scientific research of transport irradiation through heterogeneous targets.

Options includes tree thematic parts:

- Expert modes of simulation: "Normal" and "Without scattering".
- **Parameters simulation:** "Electron energy cut off", "Photon energy cut off", "Angle grouping", and "Splitting on axis X, Y, Z".
- Parameters of visualization of results: Joined cells for center and boundary, Coordinate system "normal" and "turn 90".

In the default mode "Automatic parameters" of the Software ModeSXR work, all simulation parameters are working in an optimal automatic regimes which were installed in the physical, operational and in calculation models of the Software. See Fig.16a.

All parameters of **Options** can be changed only in regime **"Manual** parameters". See Fig.16b.

5.1. Expert modes of simulation: "Normal" and "Without scattering".

<u>Mode simulation "Normal"</u>. It is standard regime with automatic choice of the parameters simulation such as <u>Electron energy cut off</u>, <u>Photon energy cut off</u>, and <u>Angle grouping</u>.

The source of photons in X-ray facility is an X-ray converter irradiated with electron beam from electron accelerator.

<u>"Normal" mode</u> characterise the full MC scheme which includes simulation: • conversion of EB into X-ray, and

• transport of X-ray beam in an irradiated target with taking into consideration the scattering effects of photons.

"Without scattering" mode characterise MC scheme which includes:

• full MC simulation the conversion of EB into X-ray, and

• MC simulation the transport of X-ray beam in an irradiated target without taking into consideration the scattering effects for photons.

Such MC simulation the transport of X-ray beam in an irradiated target without taking into consideration the scattering effects of photons is equivalent so called point kernel method without taking into consideration of the build-up factor.

😂 Options (ModeSteb 3.1 2008)	😌 Options (ModeSteb 2 1 2009)
<u>Automatic parameters</u> <u>Manual parameters</u>	Automatic narameters
Parameters of visualization of results	Decementers of visualization of visualization
O Coordinate system : normal O Coordinate system : tum 90	Coordinate system : normal Coordinate system : turn 90
Joined cells for center 10 Joined cells for boundary 10	Joined cells for center 40 Joined cells for boundary 20
Parameters of simulation	Parameters of simulation
El. energy cut off [MeV] Splittings on axis X 100	EI. energy cut off [MeV] 0,1 Splittings on axis X 10
Ph. energy cut off [MeV] 0,02 Splittings on axis Y 100	Ph. energy cut off [MeV] 0,02 Splittings on axis Y 100
Angle grouping 0,05 Splittings on axis Z 100	Angle grouping 0,05 Splittings on axis Z 10
Expert modes of simulation	Expert modes of simulation
Normal C Without scattering	Normal O Without scattering
Save data and close this window	Save data and close this window

Figs.16a, b. Main form of "Options" for enter input data for simulation. a) default mode "Automatic parameters". b) regime "Manual parameters".

5.2. Parameters of visualization of results.

5.2. 1. "Joined cells for center and boundary" define the number of cells, which were combined in the Center or Boundary of irradiated layer at calculation and visualization of 2D dose distribution.

The cells are combined in direction transversely to axis of X-ray dose distribution visualization.

5.2. 2. Coordinate system "normal" and "turn 90".

Under visualization of results, regime "turn 90" rotate the Coordinate system for the irradiated target on 90 degree around axis Z in comparison with regime "normal".

Regime "turn 90" is working only under visualization of **2D** absorbed dose distribution.

At visualization of simulation results in regime Coordinate system "normal", the 2D absorbed dose distribution is presented along "layer width". At visualization of simulation results in regime Coordinate system "turn 90", the 2D absorbed dose distribution is presented along "layer length". **5.3.** <u>Parameters simulation:</u> Electron energy cut off, Photon energy cut off, Angle grouping, and Splitting on axis X, Y, Z.

• Change of simulation parameters Electron energy cut off, Photon energy cut off, and Angle grouping can be used for scientific researches of transport irradiation through heterogeneous targets.

Note. In all above the Expert modes of simulation "Normal", "Without scattering", parameters simulation such as Electron energy cut off, Photon energy cut off, Angle grouping are automatic installed.

• Parameters simulation "Splitting on axis X, Y, Z" are used for the choice of optimal value of 3D grid for target layer at analysis of 3D absorbed dose distribution in this layer.

All parameters of **Options** can be changed only in regime "Manual parameters".

6. The features of output data representation

6.1. <u>Example. Configuration data for simulation of X-ray dose distribution</u> <u>in an irradiated target</u>

The Main form of the Software ModeStXR is presented in Fig.1. Example of target parameters data, for which simulation and preparation of output data will be made, is presented in Fig.17. Position of target on a conveyer platform is presented in Fig.18.

Full configuration data which are used at simulation are presented in Fig.19. X-ray converter structure is presented in Fig.20.

😇 ModeStxr 3.1 (2008) 💶 🗖 🗙	韋 Target and cover	(ModeStxr 3.1 20	08)						×
File Options Help About	Number of packages	Multi - Target Distance between targets	0,01	<u>Orienta</u> © Ve	ation C ertical C	Along the s Along the c	canning axis onveyor axis	s © No s O Tu	rmal displacement rn on 90 deg
Scan	Width of t	Current layer	6		Delete	Insert		Clear	
Converter	40,01 r	Laver Thickness	1	2	3	4	5	6	
	Stack length g	Width	40	- 40 2.7	40	40	40	40	
Target	20 t	Polyethylene	Z W	Z W	Z W	Z W	Z W	Z W	
	<u>2D registration</u> package + layer	PMMA Carbon	8 16	13 1	20 1	8 16	6 72 8 80	6 60 8 32	
Stop	P L 1 1 1 2	Birchwood Cellulose Soft Tissue							
16:40:42	1 3								
start 14:49:46 finished 14:51:24	1 5 C	Density	1		Poliystyrene PMMA	_	☑ List □ Tab	le T	Opened cover
View results after simulation	I 3D calculation e	Cover thickness	0,5		Carbon Birchwood Cellulose		3	0. muun h auf bi	07 ment
Open and view results from file	3D registration r	Additional cover	D		Soπ Hissue Water Teflon Aluminum		Rows	1 1 6 7	2 pan
Comparison Dosimetry	P L 1 5				Iron Another mate	rial 💌		8 8	0
Monte Carlo successfuled				21					
	Inickness, width, ad	ditional cover [cm]; L	vensity (g/cm	3]		8	save data ar	id close this wi	ndow

Main form of the Software ModeStXR









(Modelling of an irradiation of packages (-ray) ource: Pulsed regime = No;Average current = 200,000 Spectrum: MonoEnergy = Yes; Spectrum = No; Energy = 5,000 Angular spread: MonoDirect = Yes; Angular spread = No Space spread: Point beam = No; Distribute beam = Yes; Beam diameter = 4,000; Full width on half maximum = 1,000 Scanning system: Conveyor speed = 1,000; Conveyor width = 100,000; Scanning frequency = 10,000; Scanning hom height = 100,000 Scan-conv. distance = 65,000; Scanning width = 60,000; Y angle of target = 0,000; X angle of target = 0,000 Non-diverging beam = No; Triangular scanning = Yes; Default mode = Yes; Custom mode = No me: Packages = 1; Layers in each package = 6; Width of packages = 40,010; Stack length = 20,000 Distance between targets = 0,010 Target orientation along scanning axis; Normal target displacement ((Layer;Thickness;Width;Density);(1; 5,0000; 40,0000); (2, 5,0000); 40,0000); 2,0000); (3; 5,0000; 40,0000; 2,0000); (4; 5,0000; 40,0000; (Layer,Z:W):(1: 1,0000; 2,0000);(6: 5,0000; 40,0000; 2,0000)) ((Layer,Z:W):(1: 1,0000; 2,0000);(6: 5,0000; 40,0000; 2,0000)) ((2,0000);(4: 8,0000; 16,0000);(5: 1,0000; 2,0000));(5: 1,0000; 2,0000);(2: 6,0000);(3: 1,0000; 2,0000));(3: 6,0000);(4: 1,0000); (4: 8,0000);(4: 8,0000);(5: 1,0000; 2,0000);(5: 8,0000);(5: 1,0000);(6: 1,0000);(6: 6,0000);(4: 1,0000))) Converter: Layers = 3; Distance between scan and converter = 1,000 ((Layer;Thickness;Width;Density);(1; 0,1200; 0,0000; 16,6000);(2; 0,5000; 0,0000; 1,0000);(3; 0,2000; 0,0000; 7,9000)) ((Layer;Z;W):(1; 73,0000; 1,0000);(2; 1,0000; 2,0000);(2; 8,0000; 16,0000);(3; 26,0000; 1,0000)) The following package and layer were registrated in gotten 2D results:(P = 1, L = 1);(P = 1, L = 2);(P = 1, L = 3);(P = 1, L = 4); (P=1,L=5);(P=1,L=6); The following package and layer were registrated in gotten 3D results:Package = 1; Layer = 5 Options of the calculation: Energy cut off (Mev) = 0,050; Threshold energy (Mev) = 0,100; Number of joined cells for center = 10 Number of joined cells for boundary = 10; Splitting on (X,Y,Z) = (100, 100, 100); Angle grouping = 0,050 Calculation mode is normal; Normal coordinate system

Fig.19. Full set of configuration data which is used at simulation of an X-ray absorbed dose distribution.

D)istance	between	converter	and sca	an 1					
ements	Layer 1		Layer 2		Layer 3		Layer	4	Layer 5	;
ickness [cm]		0,12		0,5		0,2				
ensity [g/cm3]		16,6		1		7,9				
aterial	Z	W	Z	W	Z	W	Z	W	Z	W
	73	1	1	2	26	1				
Laver			8	16						
2										
Clear layer										
Clear layer						Sava	lata and		aie windo	

Fig.20. X-ray converter structure.

The functions of the converter layers are as follows:

韋 Configuration data

- Layer 1 X-ray converter plate Tantalum plate, thickness 1.2 mm,
- Layer 2 cooling agent water layer, thickness 5 mm,
- Layer 3 backing plate for absorbing of EB Fe plate, thickness 2 mm.

6.2. Output Data for 2D dose distributions

• After finish Simulation, Click the button "View results after simulation" in the Main form of the Software ModeStXR. The form "Dose distributions after MC simulation" with 2D absorbed dose distributions in graphical and tabular forms for chosen packages and layers in the Table "2D registration" will be opened (see Fig.21).

<u>Note 1.</u> On all curves of 2D dose distributions of X-ray in any target positions on a conveyer platform the dose value is the function of layer width (axis X).

<u>Note 2.</u> On all curves of 2D dose distributions of X-ray in any target position on a conveyer platform the dose value is integrated along layer thickness (axis Z).

• Additional information related to X-ray absorbed dose distributions are presented in this form:

• Dose uniformity ratio, DUR

- Average dose
- Dose minimum
- Dose maximum
- Statistical uncertainty
- Joined cells for centre and for boundary



Fig.21. Form with **2D** view of the depth dose distribution of X-ray in graphical and tabular forms for the 5th layer in the package.

Left graph - **2D view of the depth dose distribution** in the Centre of the 5th layer in the package. I.e. in the area Length/2.

Right graphs - 2D view of the dose distribution near the **Boundary** of the 5th layer with Air in plane XZ, <u>blue curve</u> - for first XZ plane in direction of conveyer motion, <u>violet curve</u> – for the back XZ plane in direction of conveyer motion (See Figs. 18 a, b).

• Click on any package _P_ and any layer _L_ number in the Table "2D registration", the

2D depth dose distributions for corresponding package and layer will be appear in the form.

In this way, you can see step by step the 2D depth dose distributions for all chosen packages and layers in the Table "2D registration".

• Click the button "Store all results to file", the results simulation in graphical and tabular forms will be stored for further analysis.

• To processing simulation results previously stored in the files, Click the button

"Open and view results from the file", in the Main form of the Software ModeStXR (Fig.1).

• The button "Prepare store results to compare" is used to select the 2D depth dose distributions for certain layer and package from simulation results

previously stored in the **files** and **to prepare their for use** in the **module Comparison**.

<u>Note.</u> The button "Prepare store results to compare" is active only after operation in the privies point.

• **To copy** the graphical depth-dose results into your document, **Click** graph either of the **Center** or **Boundary**, **Click the button** ''**To clipboard**'' and paste them to your document.

• The button "Prepare data to calculate SAL" is used for preparation of the dose map data in the chosen layer. Further, the dose map data can be used as input data in the software ModeSAL for calculation a sterility assurance level (SAL).

The software ModeSAL and ModeStXR are the simulation modulus of the RTOffice information system. Input and output data for all simulation modulus of the **RTOffice**

are self-consistent between themselves.

6.3. Output Data for X-ray spectrum

• Click the button "Additional results" in the form "Dose distributions after MC simulation" (see Fig.21.).

• The form with X-ray spectrum generated with 5 MeV electron beam in Tantalum converter (see Fig.20.) in graphical and tabular form will be opened (see Fig.22).



Fig.22. X-ray spectrum generated with 5 MeV electron beam in Tantalum converter.

6.4. Output Data for 3D view of an X-ray absorbed dose distributions

• Click the button "Analysis of the dose", the form "Dose map for corresponding layer and package " will be opened (see Fig.23).



Fig.23. Left Graph -3D view of the X-ray depth dose distributions (Dose Map, along layer length (axis Y) and along layer width (axis X)) in graphical and tubular forms for the 1st layer in 2nd package. The dose value is integrated along layer thickness (axis Z).

Right graphs: Cumulative distribution function – cdf (violet curve), and Probability density function in 1/kGy – pdf (green curve).

• To make analysis of the functions "Probability density function" and "Cumulative distribution function" you can use two Markers located under Right graphs: Marker 1 and Marker 2.

Click the button "Marker 1", enter a cursor in the plot field. Locate the vertical red line on the one point of the dose axis by clicking mouse in the chosen point.

Click the button "Marker 2", enter a cursor in the plot field. Locate the vertical red line on the second point of the dose axis by clicking mouse in the chosen point.

The plot will be separated with markers on three parts accordingly with scheme near the **button "Calculation"**.

Click the button "Calculation".

The integral of function "pdf" for the three parts will be appeared in the right downside of the "Dose map" form.

• Additional information related to 3D view of an X-ray absorbed dose distribution in the selected layer are presented in the form:

- Average dose
- Effectiveness
- Dose uniformity ratio

6.5. Output Data for 3D dose calculation

• Click the button "Show 3D results" in the Form with 2D depth dose distribution, the form of "Results of 3D calculation" will be opened for analysis of 3D absorbed dose distribution for the 5th layer in the package. (See Fig.24).

This layer was enter as input data in the Target example for simulation. (See Fig.17).



Fig.24. The form of "**Results of 3D calculation**" for analysis of **3D** absorbed dose distribution in the 5th layer of the package.

3D absorbed dose distribution of X-ray for any target layers can be analyzed with "spokes method".

The method includes the following operations:

• the layer volume is splitted by 3D grid with bin (cell) size $\Delta V = \Delta X \cdot \Delta Y \cdot \Delta Z$. Where ΔX =Width/ N(x), ΔY =Length/N(y), ΔZ = Thickness/ N(z).

N(x), N(y), N(z) – the number of splitting along the Layer Width (axis X), Length (axis Y) and Thickness (axis Z) respectively.

• the "spokes" can cross over the layer in any point of its surface in directions of axis X, axis Y, and axis Z perpendicularly to planes of a layer .

• the absorbed dose distribution is calculated in the "spokes" volume in directions of axis X, axis Y, and axis Z.

- the "spoke" volume (size) in directions of axis X, $V(X) = Width \cdot \Delta Y \cdot \Delta Z$
- the "spoke" volume in directions of axis Y, $V(Y) = \text{Length} \cdot \Delta X \cdot \Delta Z$
- the "spoke" volume in directions of axis Z, $V(Z) = Thickness \cdot \Delta X \cdot \Delta Y$

• at calculation the dose distribution along spokes, the absorbed dose averaging in each splitting point along spoke is realized in volume $\Delta V = \Delta X \cdot \Delta Y \cdot \Delta Z$.

Example of target layer with grid and spokes is presented in Fig.25. Layer is located on a conveyer platform.

Spoke A cross over a layer thickness along **axis Z**. **Spoke B** cross over a layer length along **axis Y**. **Spoke C** cross over a layer width along **axis X**.



Fig.25. Target layer with grid and spokes located on a conveyer platform.

For above example (see Figs. 2 and 24) all geometrical characteristics (Thickness, Width, and Length) and splitting along axis X, axis Y and axis Z for the 1st layer in 2nd package are presented in Fig.24 (right upside).



Fig.26. The form of "**Results of 3D calculation**" for analysis of **3D** absorbed dose distribution.

The sequence of operations to calculate an absorbed dose distribution along any spokes is the following (see Figs. 24 and 26):

- Select and Click on direction of the "Spoke along axis X, Y, or Z". Selected direction will be painted in brown colour.
- For example, Chosen direction is "Spoke along axis Z". (see Fig. 26).

For X and Y directions the possible values of coordinates in the XY plane will be appeared.

The cells number along axis X are in the range from 1 to 40.

The cells number along axis Y are in the range from 1 to 50.

The cells number along axis Z are in the range from 1 to 100.

Maximal number splitting cells along any axis is 100.

• Enter the number of cells in the range from 1 to 40 into window "X value (1-40)".

• Enter the number of cells in the range from 1 to 50 into window "Y value (1-50)".

• Click the button "Add curve".

The 6 windows with colour identification and for general characteristics of dose distribution for 6 curves will be opened. The general characteristics for the first dose distribution will be located in the first window frame.

The graph for the first curve for dose distribution will be appeared in the special window (see right upside Fig.26).

• Another curves for calculated dose distributions along spokes can be located in any of 6 windows. Maximal number of curves for simultaneously analysis is six.

• For this, mark by cursor any of 6 windows.

Select and Click on direction of the "Spoke along axis X, Y, or Z". Enter the number of cells in plane which will be intercrossed by spoke. Click the button "Add curve".

- You can "Delete curve", "Add curve" make "Normalization" of all curves.
- You can "Save data" for any of curves for further analysis.

• In the left frames of the "Results of 3D calculation" form, you can make the dose volume histogram analysis, DVH, in the selected layer. (see Figs. 24 and 26).

DVH is characterized by functions "pdf" and "cdf".

• To make analysis of the functions "Probability density function" and "Cumulative distribution function" you can use two Markers located under Left graphs: Marker 1 and Marker 2.

Click the button "Marker 1", enter a cursor in the plot field. Locate the vertical red line on the one point of the dose axis by clicking mouse in the chosen point.

Click the button "Marker 2", enter a cursor in the plot field. Locate the vertical red line on the second point of the dose axis by clicking mouse in the chosen point.

The plot will be separated with markers on three parts along **axis Dose**. Click the button "Calculation".

The analysis of **DVH data results** for the three parts will be appeared in the left downside of the form "**Results of 3D calculation**".

• You can save the analysis of DVH data by use the button "Save DVH data".

7. <u>Comparison of simulation results</u>

Module "Comparison" is intended for the scientific analysis and comparison of calculated data of 2D absorbed dose distributions in an irradiated multilayer target.
Click the button "Comparison" in the Main form of the Software ModeStXR (See Fig.1).

The form of "Comparison of calculated curves" will be opened for analysis of calculated 2D absorbed dose distributions in an irradiated target layers (See Fig.10).

The analysis can be carried out with current calculated data or data calculated before.

• **Choose** for analysis the calculated curve in the frame under the window "Number of the curve". For that, tick the chosen curve with cursor.

There are the following variants of calculated curve for the choice:

- 1. "After Monte Carlo calculation" it is the results of current calculation of the dose distributions in the multilayer target.
- 2. "Prepared stored results"- it is simulation results of the 2D dose distributions which were previously stored in the files.

These results can be selected for comparison only when the following sequence operations

will be done before the selection:

• Click the button "Open and view results from the file" in the Main form of the Software ModeStEB. (See Fig.1).

The 2D dose distribution will be appeared in the form "Dose distributions after MC simulation" from the chosen file.

• Click the button "Prepare store results to compare" in the form "Dose distributions after MC simulation". (See Fig.21).

- 3. "Converted dosimetric file" it is result which was calculated and saved for the EB dose distribution along any spokes in the form of "Results of 3D calculation" and further converted through the block "Dosimetry". (See Fig.24).
- 4. "After dosimetric block" it is results for dose distributions which were obtained and saved after processing of dosimetric films with the block "Dosimetry".

• Select the position of dose distribution in the Center or Boundary of irradiated layer for the chosen curve of 2D dose distribution.

• Select the number of package _P_ and number of layer _L_ in the Registration table.

• Enter the value X in cm in the window "X position" for the chosen curve, if it is necessary. X position is characterized the displacement of curve of 2D dose distribution along axis X relatively the value X=0. In the default mode the value of "X position" = 0.

• Select by cursor the any of 6 columns of the table in the bottom part of the form the "Comparison of calculated curves". The chosen column number will be automatically entered to the window "Number of the curve".

Click the button "Load curve from X position".

The characteristics of the 2D dose distribution curve will be appeared in the chosen column. And the graph of the 2D dose distribution curve will be appeared in the graph area.

In a such way you can enter for analysis up to 6 curves of 2D dose distributions in the graph area. (See Fig.27).

You can "Delete selected curves" and make for all curves "Normalization". (See Fig.27).



Fig.27. The form of "Comparison of calculated curves". Example of 2D dose distributions for some layers calculated along layer width for multilayer target with composition presented in Fig.17.

The function of button "Compare marked curves" allows to make comparison of 2D dose distributions for 2 any curves to obtain the values of differential and integral deviations in % between compared curves. (see Fig. 27).

For that, select the numbers of 2 compared curves and click the button "Compare marked curves".

• **To copy** the results comparison into your document, **Click** the graph by right mouse button.

Then Click the button "Plot mode 2D/3D", if it is necessary, and then Click the button "Plot to clipboard" and paste them to your document.

8. Dosimetry module

Block "**Dosimetry**" is intended for processing of dosimetric films with experimental data and to prepare data for "**Comparison**" module.

• Click the button "Dosimetry" in the Main form of the Software ModeStXR (See Fig.1). The form of "Preparing of experimental dosimetric data" will be opened for analysis of calculated and experimental data of 2D absorbed dose distributions in an irradiated target (See Fig.28.a).



Figs. 28 a, b. The forms for "Preparing of experimental dosimetric data".

• Load a text file with experimental data from hard disk. A file may contains three or two columns (X and Y, or X, Y1, Y2). (See Fig.28 b). Loaded data are showing onto the plot and into a grid and the buttons Move and Invert, Cut and Scale, Convert data for Comparison appear. (See Figs.29 a, b).



Figs. 29 a, b. The forms for "Processing of experimental dosimetric data".

• To move selected curve to left or invert one you need to use the control panel that will open when the button Move and Invert is pressed. To save changes, press the button Apply.

• Click the button Cut and Scale, to cut and scale curves data.

• To cut a part of curves you mark by a circle Marker 1 and move a mouse pointer to the plot. In this point a vertical red line appears onto plot. You move it and place by left mouse clicking. It is a first limited line. You make the same with Marker 2 and place a second red line. (See Fig.29. a).

You must scale the curves and press **Apply**. A part of curve placed between two red lines will saved, a plot will repaint and a grid will rewrite.

The button Convert data for Comparison and its control panel provides the data for Comparison block. If you have made a scale of curves the pressing of Apply creates a new red curve onto plot and show new data in the grid.

(See Fig.29. b).

These data may be stored to a file with using Save as "*.flm" file. You can work with a film file if load it.