nSSF

A Windows software for the determination of neutron self-shielding correction factors

(Draft) User Guide

Current version: v0.9 (Beta)

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by

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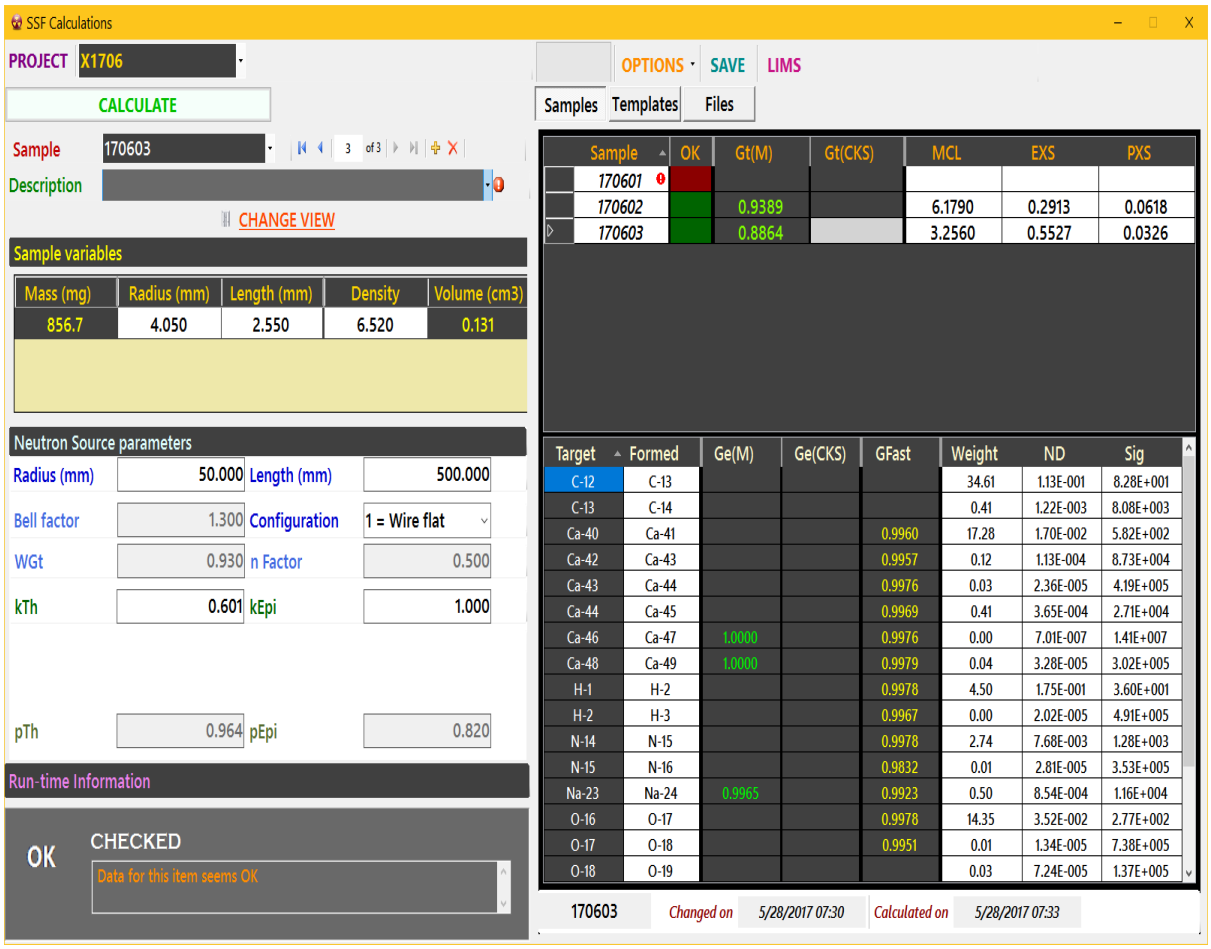
The MatSSF open-source (FORTRAN) code was developed by Dr. Andrej Trkov and it is available at the International Atomic Energy Agency (IAEA) website:

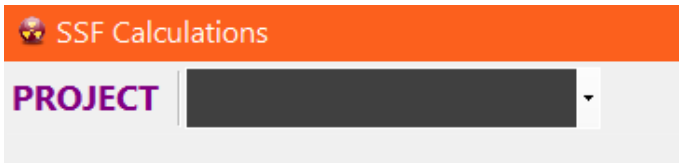
https://www-nds.iaea.org/naa/matssf/

The latest version that is bundle to this software dates February 2016


SSF Calculations
PROJECT X1706
CALCULATE
Sample 170603
Description
CHANGE VIEW
Sample variables
Mass (mg) 856.7
Radius (mm) 4.050
Length (mm) 2.550
Density 6.520
Volume (cm3) 0.131
Neutron Source parameters
Radius (mm) 50.000
Length (mm) 500.000
Bell factor 1.300
Configuration 1 = Wire flat
WGt 0.930
n Factor 0.500
kTh 0.601
kEpi 1.000
pTh 0.964
pEpi 0.820
Run-time Information
OK
CHECKED
Data for this item seems OK
OPTIONS
SAVE
LIMS
Samples
Templates
Files
Sample OK Gt(M) Gt(CKS) MCL EXS PXS
170601
170602 0.9389 6.1790 0.2913 0.0618
170603 0.8864 3.2560 0.5527 0.0326
Target Formed Ge(M) Ge(CKS) GFast Weight ND Sig
C-12 C-13 34.61 1.13E-001 8.28E+001
C-13 C-14 0.41 1.22E-003 8.08E+003
Ca-40 Ca-41 0.9960 17.28 1.70E-002 5.82E+002
Ca-42 Ca-43 0.9957 0.12 1.13E-004 8.73E+004
Ca-43 Ca-44 0.9976 0.03 2.36E-005 4.19E+005
Ca-44 Ca-45 0.9969 0.41 3.65E-004 2.71E+004
Ca-46 Ca-47 1.0000 0.9976 0.00 7.01E-007 1.41E+007
Ca-48 Ca-49 1.0000 0.9979 0.04 3.28E-005 3.02E+005
H-1 H-2 0.9978 4.50 1.75E-001 3.60E+001
H-2 H-3 0.9967 0.00 2.02E-005 4.91E+005
N-14 N-15 0.9978 2.74 7.68E-003 1.28E+003
N-15 N-16 0.9832 0.01 2.81E-005 3.53E+005
Na-23 Na-24 0.9965 0.9923 0.50 8.54E-004 1.16E+004
O-16 O-17 0.9978 14.35 3.52E-002 2.77E+002
O-17 O-18 0.9951 0.01 1.34E-005 7.38E+005
O-18 O-19 0.03 7.24E-005 1.37E+005
170603
Changed on 5/28/2017 07:30
Calculated on 5/28/2017 07:33

Making a Project

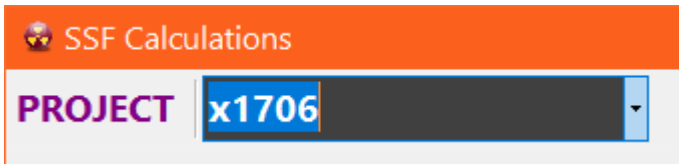
1. In the “Project” box as shown in the figure, type in the label name of the project your would like to create.



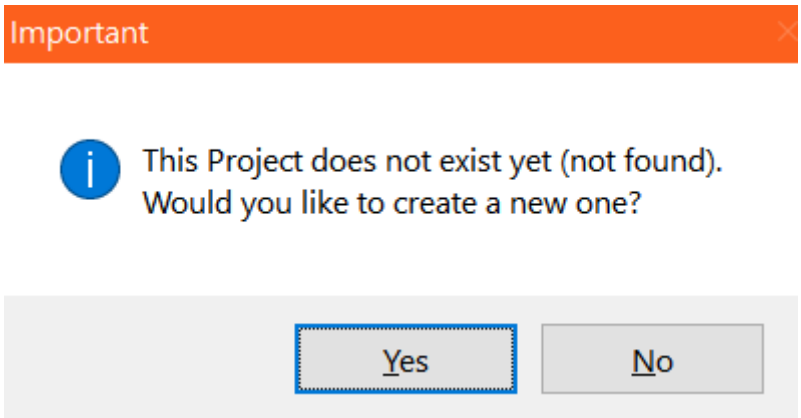
You could type for instance:

“X1706”

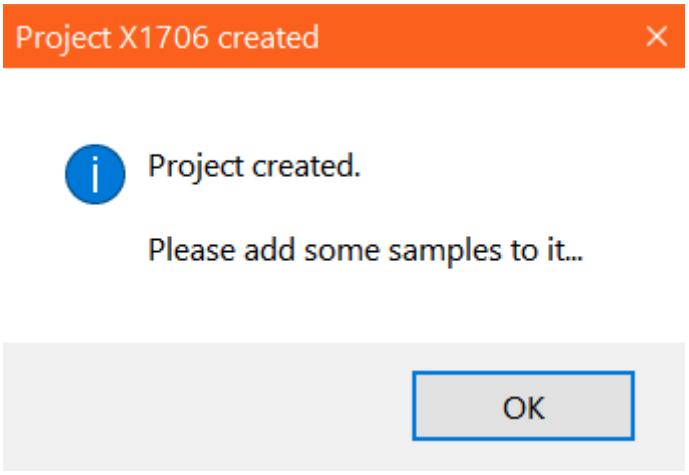
as a nemonic for project **X** on the year **2017** and month **6**.



2. Press **ENTER** to create the project. A confirmation dialog will show up.

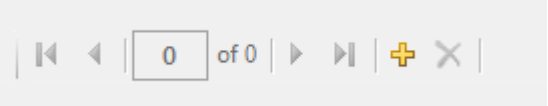


3. After clicking **YES** a confirmation dialog will show up.



Adding samples

4. In order to add a sample, employ the yellow **Plus** (**+) Button** located in the "**Navigation Bar**"

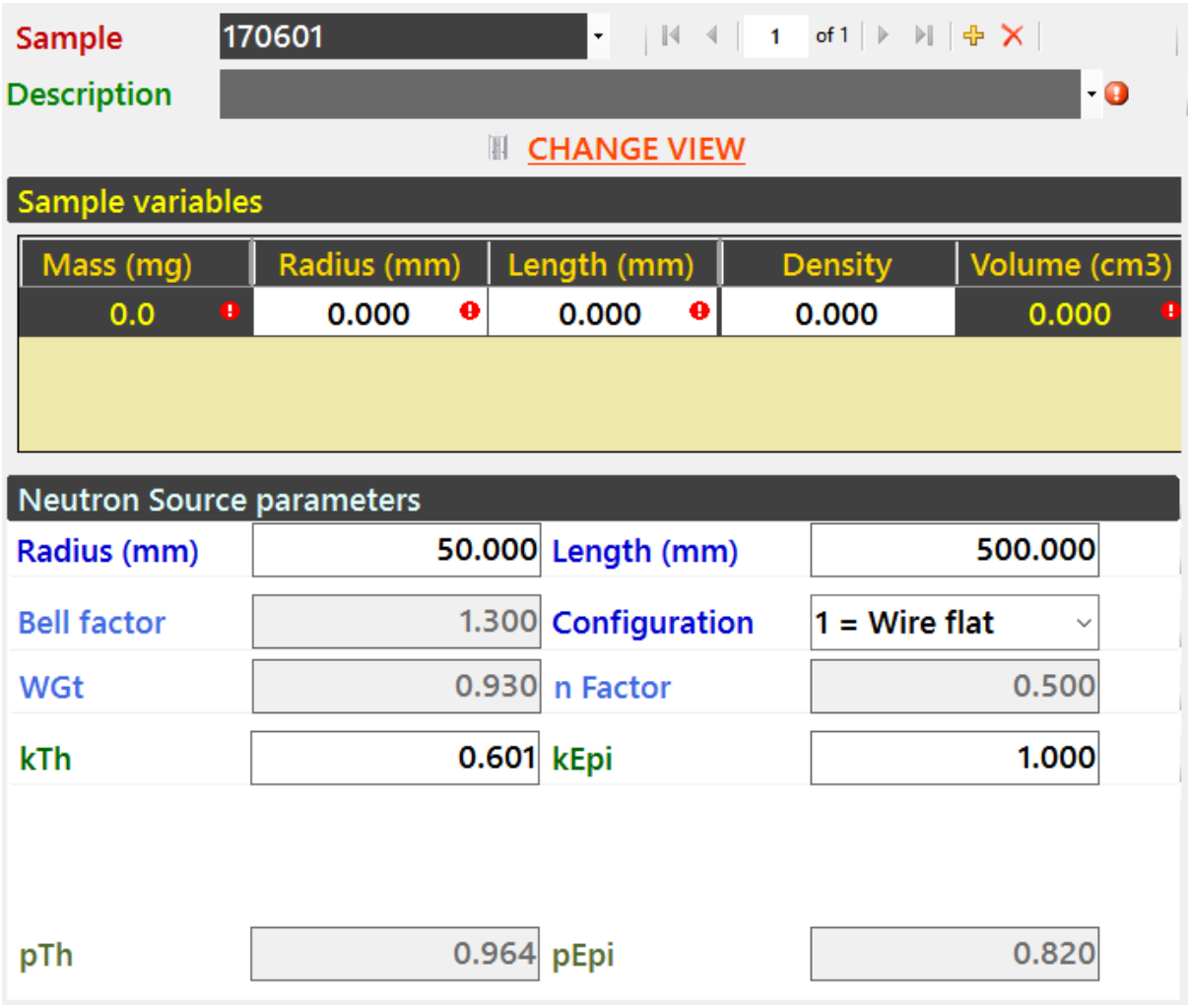


5. A new sample is added and its particular sample information is displayed at the application left-hand side panel:

On top you will identify the typical **Sample variables** for cylindrical samples:

Radius (in mm), **Length** (in mm), **Density** (in g/cm^3), **Mass** (in mg) and **Volume** (in cm^3).

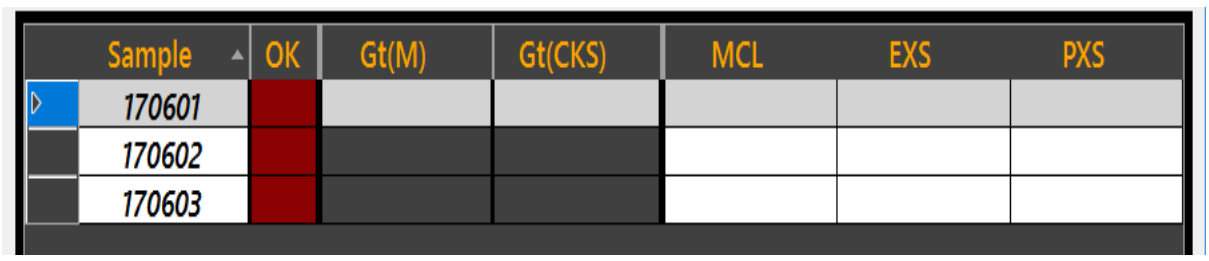
A **Grey** cell indicates that the value is read-only and will be automatically calculated each time each of the **White** cell parameters are **validated.**



For instance, the Mass is recalculated each time the Radius, Length or sample Density is modified and validate**d.**

6. Type in the desired sample value in a given White cell **and press ENTER to validate the value.**

7. Add more samples to your project. These samples will appear in the application right-hand panel (see the figure below).



You can navigate/select which sample you would like to modify by selecting any cell of the respective data row → 

The top grid will also display overall sample results from the calculations, i.e.:

- **Gt(M)** refers to the **Thermal** neutron self-shielding correction factor according to the MatSSF method. [1,2]

- On the other hand the **Gt(CKS)** value refers to the **Thermal** neutron self-shielding correction factor according to the Chilian-Kennedy Sigmoid method. [3–6]

Other parameters

MCL	EXS	PXS
6.1790	0.2913	0.0618
3.2560	0.5527	0.0326

- The **MCL** corresponds to the **Mean-chord length (in cm).**

- The **EXS** value corresponds to the **Escape cross-section (in cm^{-1}).**

- The **PXS** value corresponds to the **Potential cross –section (in cm^{-1}).**

The bottom sample grid on the right-hand side panel will show the sample specific results for the formed nuclei (available in the library):

Target	Formed	Ge(M)	Ge(CKS)	GFast	Weight	ND	Sig

- **Ge(M)** refers to the **Epithermal** and **GFast(M)** refers to the **Fast** neutron self-shielding correction factors according to the MatSSF method. [1,2]

- On the other hand the **Ge(CKS)** value refers to the **Epithermal** neutron self-shielding correction factor according to the Chilian-Kennedy Sigmoid method. [3–6]

- The **ND** value corresponds to the **Nuclei or Isotope Density** (in 10^{24} $i.cm^{-3}$).

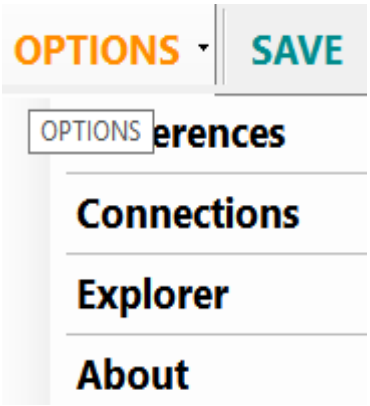
- The **Sig** value corresponds to the **Macroscopic cross-section** (in barns).

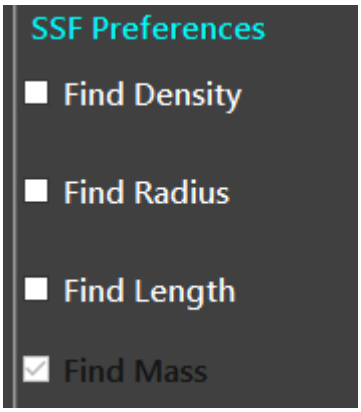
- The **Weight** corresponds to the **% content** of a given isotope in the sample.

Other sample information is available on the bottom of this panel, as shown below:

IMPORTANT: PREFERENCES MENU

It is possible to change which sample parameter gets automatically recalculated by accesing the "**Preferences**" menu located in the "**Options**" menu (see the figure below)





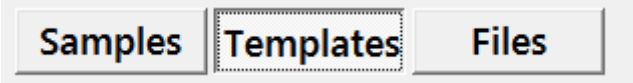
By clicking "**Preferences**" a pop-up menu will appear. You can choose wether you would like to automatically recalculate the **Density**, the **Radius** or the **Length** of the sample by chekcing these boxes. In order to automatically recalculate the sample **Mass**, you need to uncheck all these boxes.

Close the **Preferences** menu.

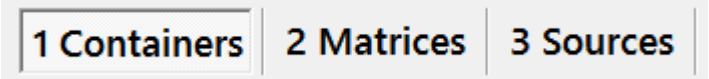
Templates

One of the main ideas of this program is to be able to reuse sample "**Matrices**" (or Compositions), "**Containers**" and **neutron** "**Sources**" that are already present in the database.

8. Acces the "**Templates**" right-panel according to the following figure:

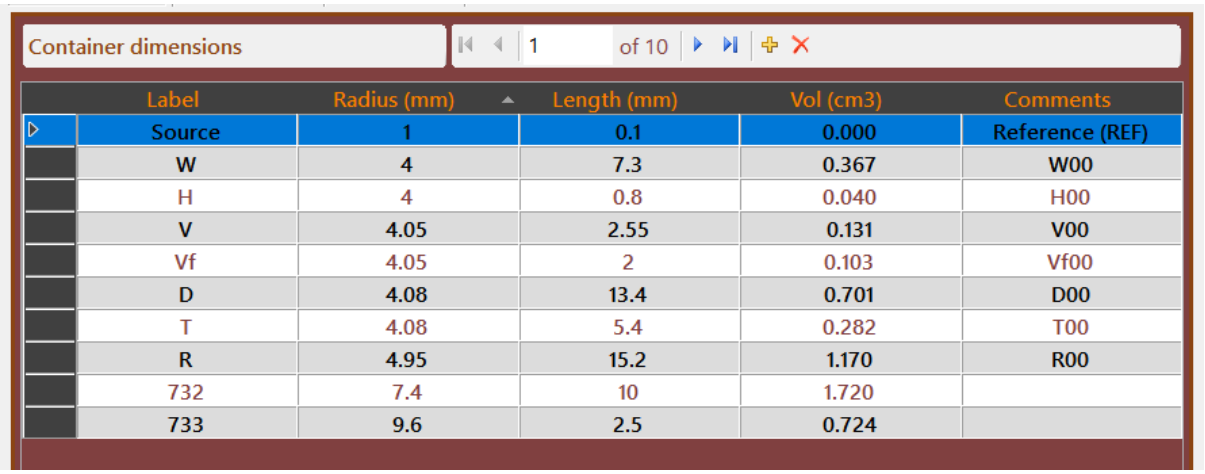


Under this panel you can access 3 different types of Templates.



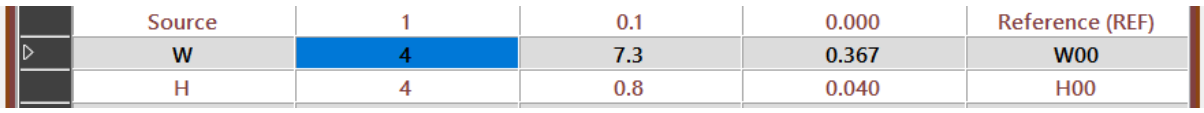
Containers

9. By selecting "Containers" the user can acces a templates list of different containers to choose.



Label	Radius (mm)	Length (mm)	Vol (cm3)	Comments
Source	1	0.1	0.000	Reference (REF)
W	4	7.3	0.367	W00
H	4	0.8	0.040	H00
V	4.05	2.55	0.131	V00
Vf	4.05	2	0.103	Vf00
D	4.08	13.4	0.701	D00
T	4.08	5.4	0.282	T00
R	4.95	15.2	1.170	R00
732	7.4	10	1.720	
733	9.6	2.5	0.724	

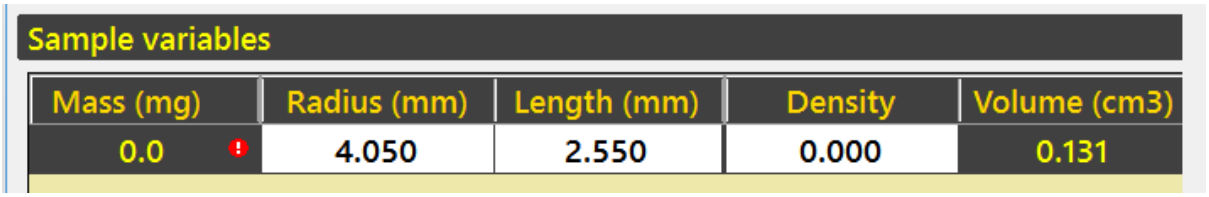
10. It is also possible to create more containers and/or modify their values by selecting the respective cell and typing its value.



Source	1	0.1	0.000	Reference (REF)
W	4	7.3	0.367	W00
H	4	0.8	0.040	H00

11. In order to ASSIGN the (template) container dimensions to the sample, DOUBLE-CLICK on the respective row header of the container 

The **Radius** and **Length** values of the selected container will replace the Radius and Length values of the sample:



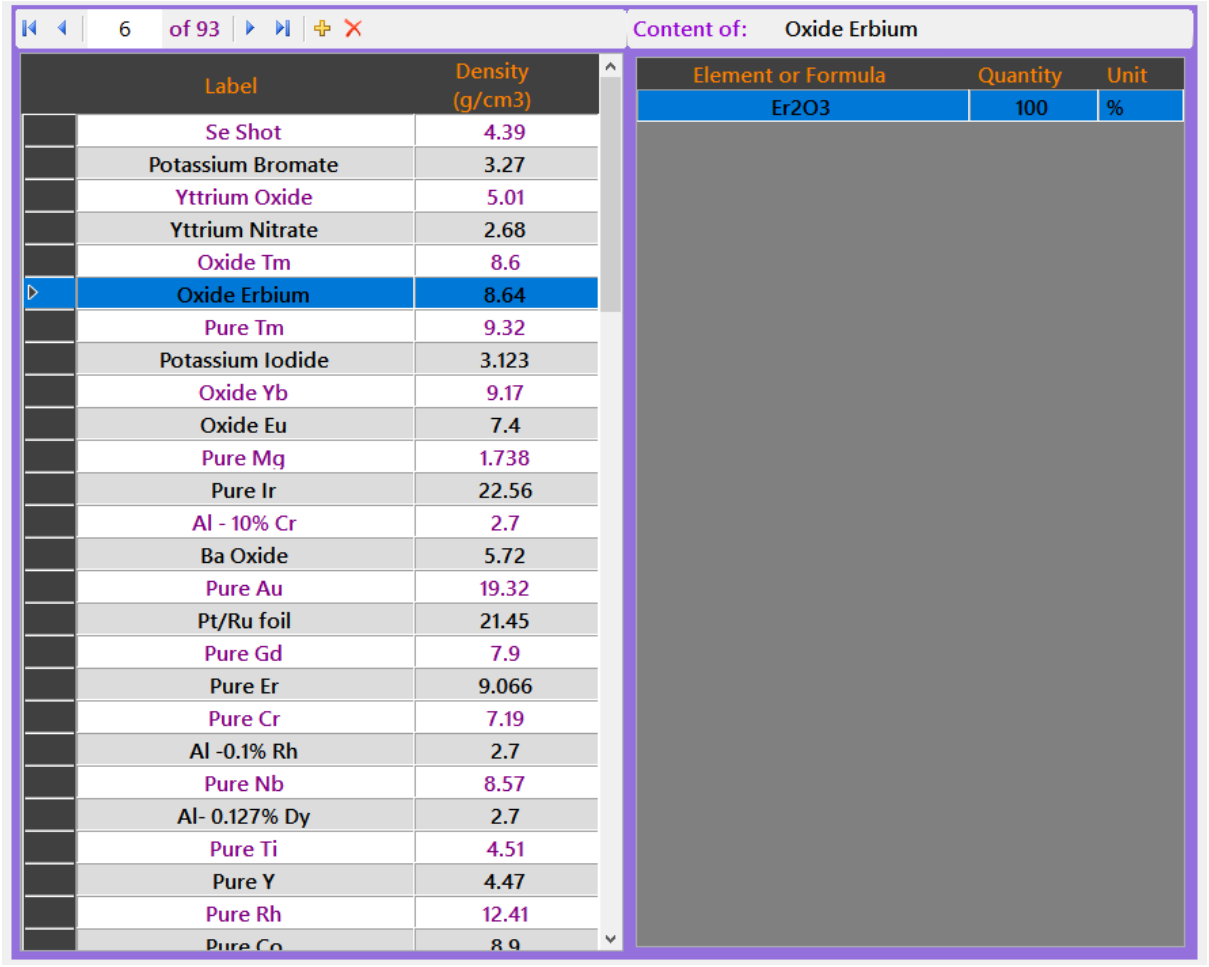
IMPORTANT

Modifying the values of a given template item **will not automatically modify** the values in the respective associated sample. This is done in order to ensure that each sample parameter can be modified later at will by the user. The template values are only meant to be cloned each time the user double-clicks on the respective item**.**

However, the templates are internally linked (associated) to the respective sample. Linking is perfomed to ensure that further versions of the program will allow for restoration off the sample parameters to the default template values if the user choses to.

Matrices

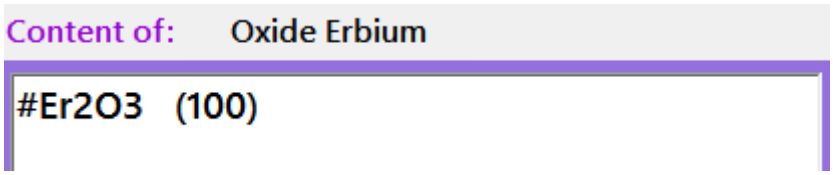
12. By selecting "**Matrices**" the user can acces a templates list of different containers to choose.



On the left-hand, a list of matrices is shown. Each matrix content can be modified in the right-hand side grid.

Editing a Matrix

13. Hover your mouse to the right-hand "**Content**" grid. The grid will be transformed into a text input box as shown in the figure below:



14. Type in the matrix content following these strict rules:

#Element (%Content)

or,

#Formula (%Content)

Examples:

#Al (50) #Fe (33.3) #Gd (16.7)

#Al2O3 (20) #Ba1O1 (60) #Mn (20)

Nota Bene: When inputting formulas, the user will need to input explicitly the number "**1**" that is typically implicit for a given formula. This is not necessary when inputting pure elements.

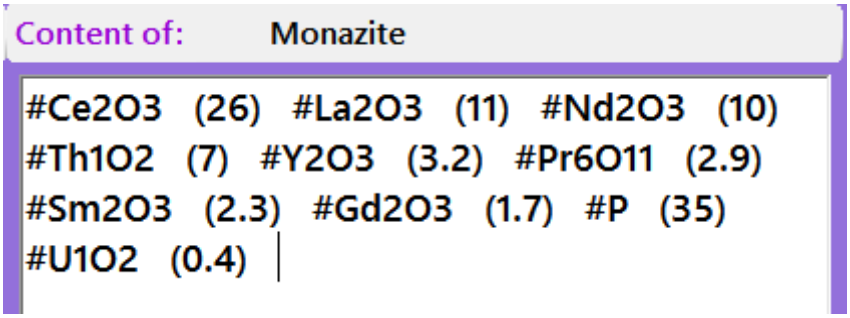
Examples:

#BaO is **incorrect**, while **#Ba1O1** is **correct.**

#Fe is **correct.**

Multi-compound single-Matrix

The program allows for multi-compoun single-Matrices such as e.g. a Monazite mineral:



When your mouse leaves the area, the matrix content grid gets updated displaying the new list of compositions (see the figure below).

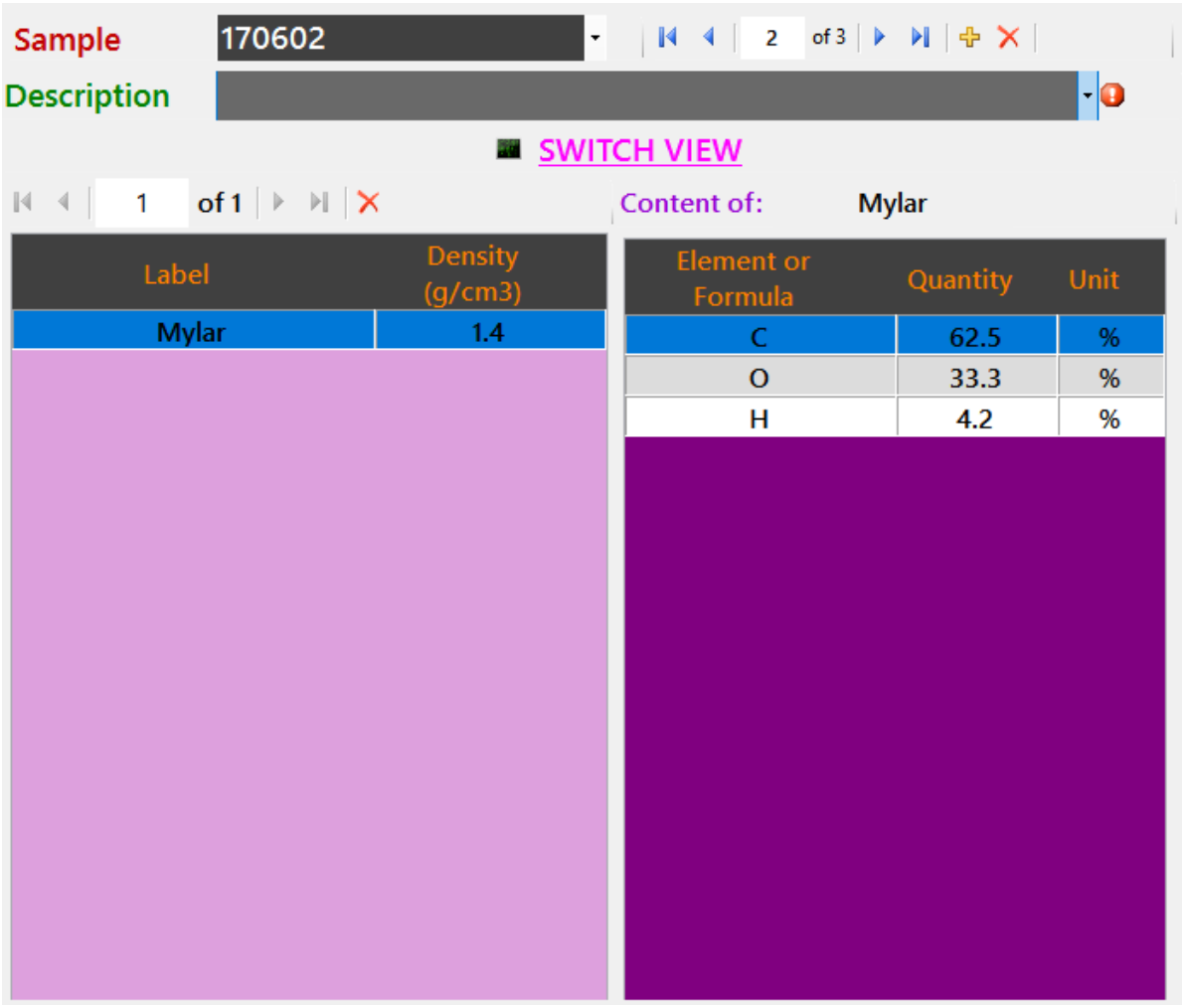
Content of: Monazite

Element or Formula	Quantity	Unit
U1O2	0.4	%
P	35	%
Gd2O3	1.7	%
Sm2O3	2.3	%
Pr6O11	2.9	%
Y2O3	3.2	%
Th1O2	7	%
Nd2O3	10	%
La2O3	11	%
Ce2O3	26	%

Adding a Matrix to a Sample

15. **In order to ADD a (template) matrix to the sample, DOUBLE-CLICK on the respective row header of the item** 

The matrix is cloned/copied into the list of sample matrices located on the main left panel. The cloned matrix will show up in the "**Composition View**" as in the following figure:



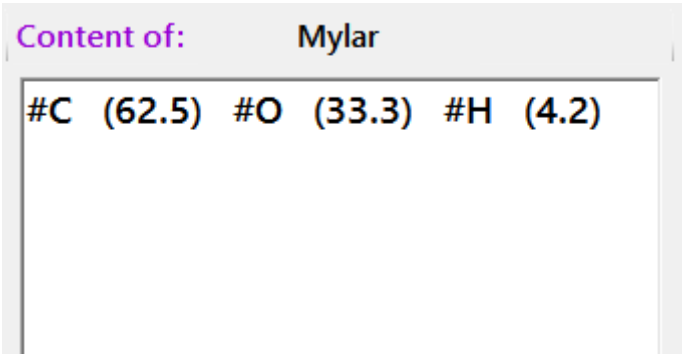
The sample and neutron source panel can be accesed back by clicking on the CHANGE VIEW button.

Nota bene: When you adopt **the first** matrix template, its **Density** value is copied to the **sample Density** and the respective Grey cell is recalculated (e.g. the Mass).

Sample variables

Mass (mg)	Radius (mm)	Length (mm)	Density	Volume (cm3)
981.1	4.080	13.400	1.400	0.701

16. Modify the content of the sample matrix as in the previous example:



IMPORTANT

You can add to the sample as many clones of template matrices as you want. However, modifying the content of a matrix associated to a sample **will not automatically** modify the content of a template matrix, and viceversa. Once again, this is to ensure that each sample can be specific and modified at will. Further program versions will allow for the option of restoration of sample values from associated template data if desired.

Still, you can modify the template matrix and re-adopt the updated values into the sample by double-clicking **again** the row header of the modified template matrix (a manual **Matrix UPDATE**).

Neutron Sources

17. By selecting “Sources” you can acces a templates list of different neutron sources configurations and dimensions to choose.

On the top grid the user can choose from a list of Neutron source “**Configurations**” and “**Dimensions**”, which are basically fixed (fundamental) neutron source parameters for a given neutron source.

Neutron source configurations

2 of 2

	Label	Prefix	Configuration	Bell Factor	WGt	nFactor	kth	kepi	pTh	pEpi
	S84	Z	1 = Wire flat	1.3	0.93	0.5	0.6449	1	0.964	0.820
▷	Y4	X	1 = Wire flat	1.3	0.93	0.5	0.601	1	0.964	0.820

Neutron source dimensions

4 of 6

	Label	Radius	Length	Vol	Comments
	S84	40	300	1,507.964	S84
	PE50	45	220	1,399.580	
	PE20	47	560	3,886.276	
▷	Y4	50	500	3,926.991	Y4
	PE200	60	340	3,845.309	
	P100	85	500	11,349.003	

These grids control the “Neutron source parameters” Sample values in the panel located at the left-hand side (see the figure below)

Neutron Source parameters

Radius (mm)	50.000	Length (mm)	500.000
Bell factor	1.300	Configuration	1 = Wire flat
WGt	0.930	n Factor	0.500
kTh	0.601	kEpi	1.000
pTh	0.964	pEpi	0.820

Methods semi-empirical parameters

On the top grid (see figure below), each paramater corresponds to a given calculation method:

	Label	Prefix	Configuration	Bell Factor	WGt	nFactor	kth	kepi	pTh	pEpi
	S84	Z	1 = Wire flat	1.3	0.93	0.5	0.6449	1	0.964	0.820

MatSSF method:

- **Bell Factor**:

- **nFactor**:

- **WGt:**

- **Configuration:**

CKS method:

- **kth:**

- **kepi:**

- **pTh:**

- **pEpi**:

18. In order to ASSIGN the (template) neutron source configuration to the sample, DOUBLE-CLICK on the respective row header of the item

For instance, if you select the row “Y4” → 

the sample in the left-hand panel will be updated with the incoming values according to the respective calculation method (as shown):

For the MatSSF method

Bell factor	1.300	Configuration	1 = Wire flat
WGt	0.930	n Factor	0.500

For the CKS method

kTh	0.601	kEpi	1.000
pTh	0.964	pEpi	0.820

IMPORTANT

The "**Prefix**" column has a special purpose. If a Project is labelled with a prefix letter present in this template list, each added sample will automatically acquire that neutron source configuration.

	Label	Prefix
	S84	Z
▷	Y4	X

Neutron source dimensions

19. **In order to ASSIGN the (template) neutron source dimensions to the sample, DOUBLE-CLICK on the respective row header of the item** 

Neutron source dimensions — 4 of 6

	Label	Radius	Length	Vol	Comments
	S84	40	300	1,507.964	S84
	PE50	45	220	1,399.580	
	PE20	47	560	3,886.276	
▷	Y4	50	500	3,926.991	Y4
	PE200	60	340	3,845.309	
	P100	85	500	11,349.003	

The following sample values in the left-hand panel will be updated with the incoming values:

Radius (mm)	50.000	Length (mm)	500.000

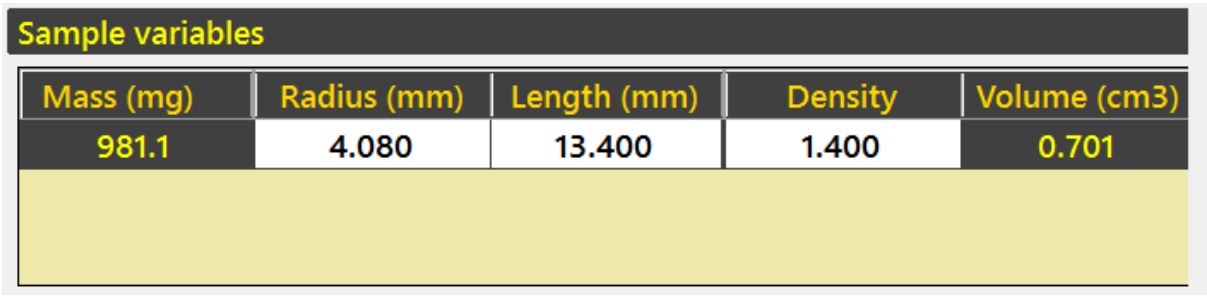
IMPORTANT

The "**Label**" column in this grid has a special functionality. If a "Neutron source dimension" label matches a "Neutron source configuration" label, then both template items are linked, and each added sample will automatically acquire that neutron source dimension as well.

	Label	Prefix
	S84	Z
▷	Y4	X

Calculations

1. Once the samples have no visible cell errors as e.g. the figure below, the user can calculate the thermal and epithermal neutron self-shielding correction factors for each sample separatedly or, in batches.

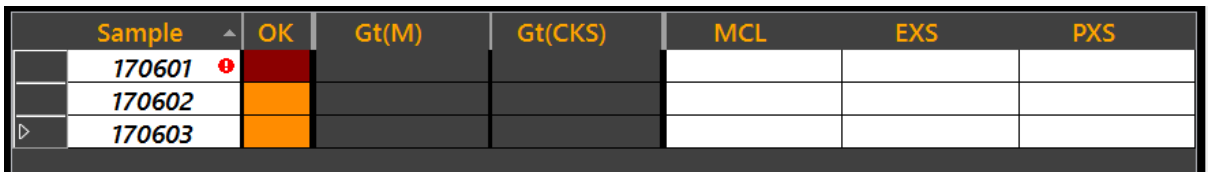


Sample variables

Mass (mg)	Radius (mm)	Length (mm)	Density	Volume (cm3)
981.1	4.080	13.400	1.400	0.701

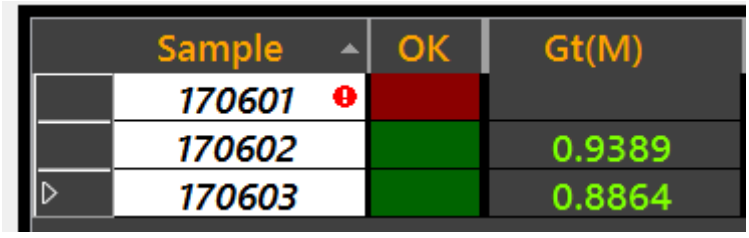
2. Click the CALCULATE button to start the calculations.

3. When the calculations start, the sample status turns **Yellow/Orange**. the samples that were rejected from the calculation process remain **Red** and an error message is attached to their sample label (see the figure below).

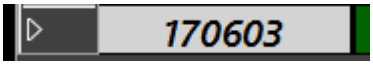


Sample	OK	Gt(M)	Gt(CKS)	MCL	EXS	PXS
170601						
170602						
170603						

4. When calculations are finished, the **thermal** neutron self-shielding correction factors are displayed and the sample status becomes **Green** (see the figure below).



Sample	OK	Gt(M)
170601		
170602		0.9389
170603		0.8864

5. To display the **epithermal** neutron self-shielding correction factors select the sample of interest → 

The bottom grid will be updated with the respective sample values for each reaction of interest.

Target	Formed	Ge(M)	Ge(CKS)	GFast	Weight	ND	Sig
Ca-44	Ca-45			0.9969	0.41	3.65E-004	2.71E+004
Ca-46	Ca-47	1.0000		0.9976	0.00	7.01E-007	1.41E+007
Ca-48	Ca-49	1.0000		0.9979	0.04	3.28E-005	3.02E+005
H-1	H-2			0.9978	4.50	1.75E-001	3.60E+001
H-2	H-3			0.9967	0.00	2.02E-005	4.91E+005
N-14	N-15			0.9978	2.74	7.68E-003	1.28E+003
N-15	N-16			0.9832	0.01	2.81E-005	3.53E+005
Na-23	Na-24	0.9965		0.9923	0.50	8.54E-004	1.16E+004
O-16	O-17			0.9978	14.35	3.52E-002	2.77E+002
O-17	O-18			0.9951	0.01	1.34E-005	7.38E+005
O-18	O-19				0.03	7.24E-005	1.37E+005
Zr-90	Zr-91	0.9549		0.9445	12.66	5.53E-003	1.79E+003
Zr-91	Zr-92			0.9904	2.79	1.21E-003	8.21E+003
Zr-92	Zr-93			0.9898	4.31	1.84E-003	5.37E+003
Zr-94	Zr-95	0.9726		0.9658	4.47	1.87E-003	5.30E+003
Zr-96	Zr-97	0.9665		0.9638	0.73	3.01E-004	3.29E+004

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6. Select for instance another sample, the bottom grid is automatically updated showing the values for that sample.

Target	Formed	Ge(M)	Ge(CKS)	GFast	Weight	ND	Sig
C-12	C-13				61.78	4.34E-002	8.52E+001
C-13	C-14				0.72	4.69E-004	8.30E+003
H-1	H-2			0.9992	4.20	3.51E-002	9.05E+001
H-2	H-3			0.9985	0.00	4.04E-006	9.65E+005
O-16	O-17			0.9991	33.21	1.75E-002	2.19E+002
O-17	O-18			0.9974	0.01	6.67E-006	5.85E+005
O-18	O-19				0.08	3.60E-005	1.08E+005

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