Installation

The RSD2013 software is compiled to run on a Windows platform. It mainly consist out of two executables: `RSD2013_GUI.exe` and `RSD2013.exe`. The first executable is the graphical user interface (GUI) which creates the input files and can start up the RSD2013 simulations. The second executable is the effective simulation program. After generating an input with the GUI or manually, you can run `RSD2013_GUI.exe` on the command line to perform the simulation.

Installation of the RSD2013 software is easy. Simply unpack the compressed zip file to a location of your choice and you are ready to use the software. The directories `icons` and `templates` should be left intact. Renaming the `RSD2013.exe` executable will make running simulations through the GUI impossible.

Overview

The RSD2013 software is developed to simulate the reactive sputter process of a DC magnetron. It's focus is on the possible hysteresis curve of this process. To this end, it solves the equations of the RSD2013 model, as can be found in following reference. The nomenclature of the variables used here corresponds with the one of this reference.

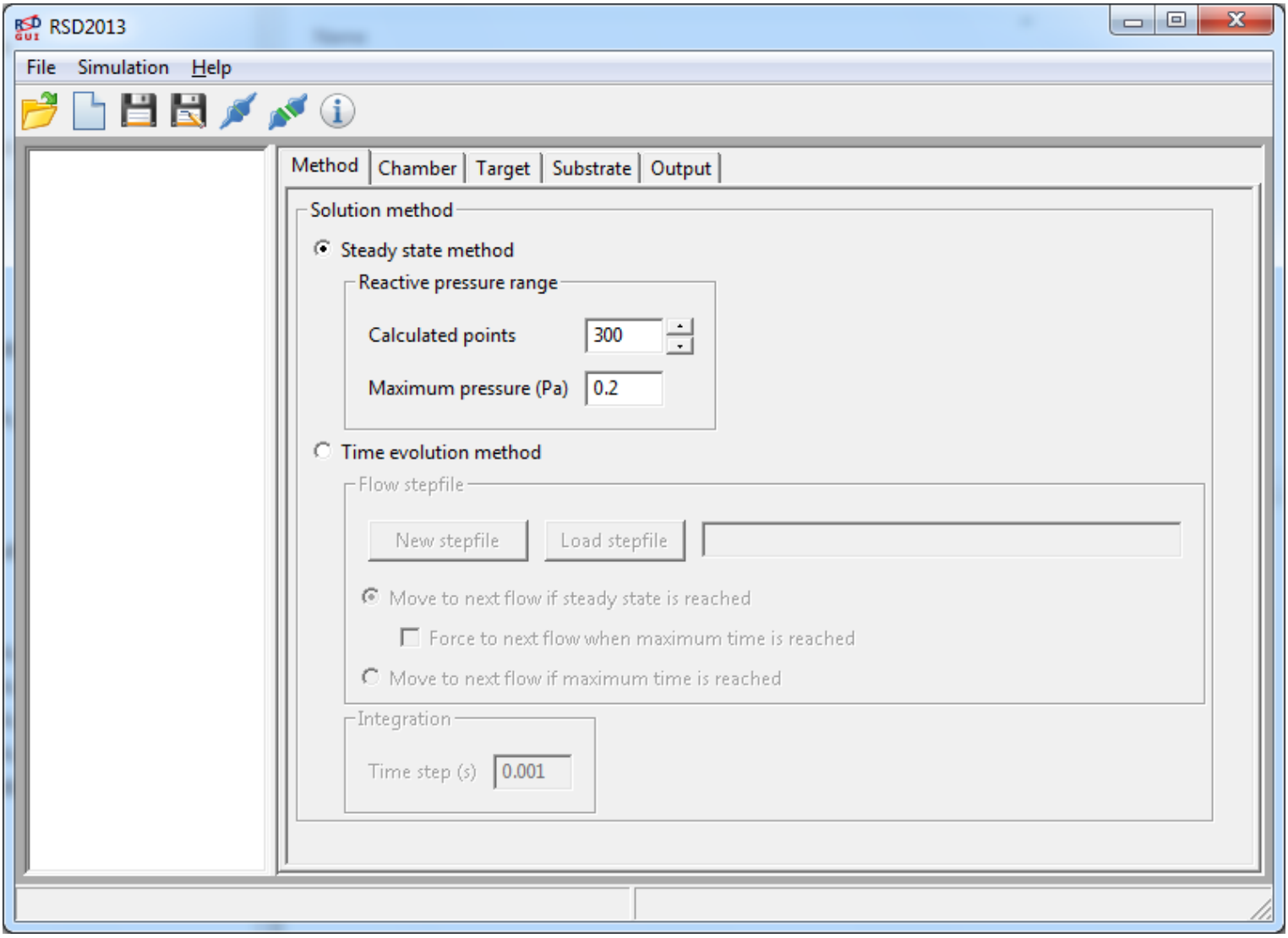
The RSD model calculates following variables:

- the pressure P_r of the reactive gas in the system
- the compound θ_r, chemisorbed θ_c and metal θ_m fractions on the target surface
- the compound θ_s and metal fractions on the substrate surfaces
- the metal concentration n_M in the target subsurface region
- the compound concentration in the target subsurface region which is directly derived from n_M
- the non-reacted implanted reactive gas concentration n_R in the target subsurface region
- the consumptions Q_t of reactive gas by the target
- the consumptions Q_s of reactive gas by the substrate
- the amount of reactive gas Q_p pumped away by the vacuum pump
- the amount of reactive gas Q_{in} introduced into the vacuum chamber

To calculate these variables, the RSD model needs several input variables. These input variables are clarified throughout the following sections.

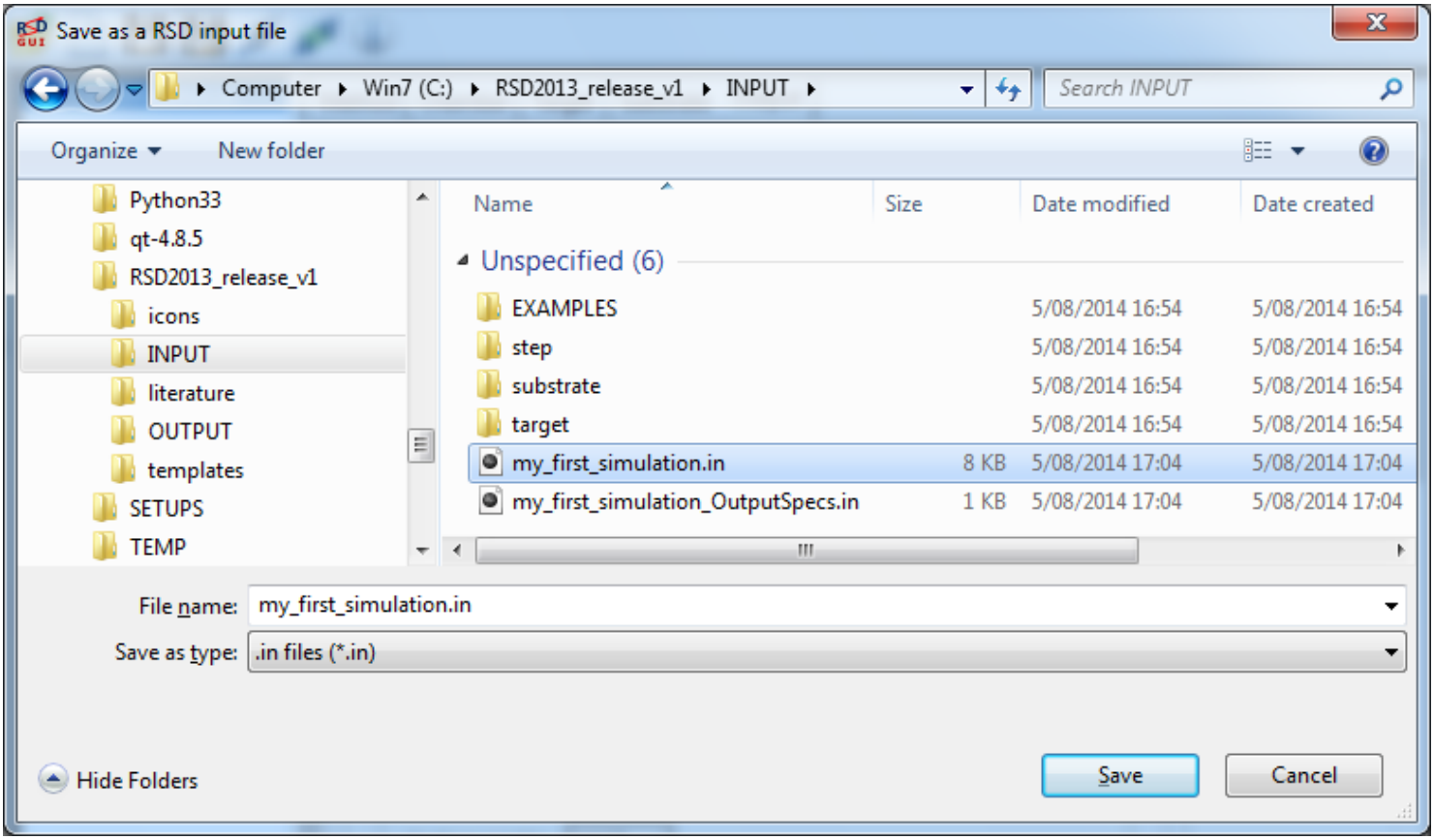
Quick start

To run a first RSD simulation, you just double click the GUI executable `RSD2013_GUI.exe`. By default a complete input is specified in the window tabs `Method`, `Chamber`, `Target`, `Substrate` and `Output`.



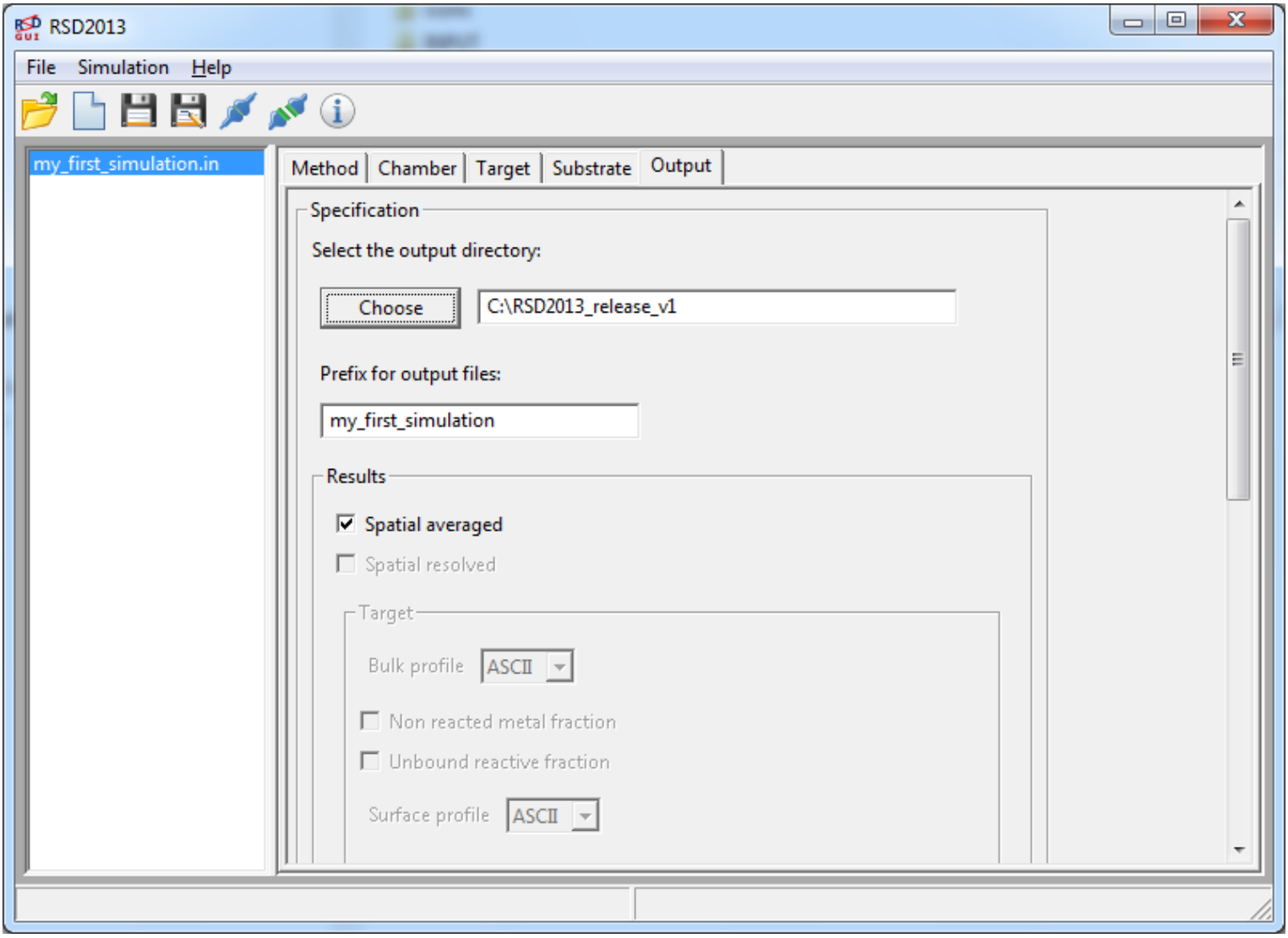
Default input.

To run this default simulation, you first have to save the simulation input. By choosing `File` > `Save as ...` in the menu bar or pressing on the icon  , a window pops up to specify a saving location and a name for the main input file. Choose as location the `INPUT` directory under the RSD program folder, and as name, for example, `my_first_simulation.in`. Press the `Save` button. Two input files will be created, namely `my_first_simulation.in` and `my_first_simulation_OutputSpecs.in`. The first file is the main input file, while the second file is the input file specifying the generated output. These specifications are defined in the window tab `Output` under `Results`.



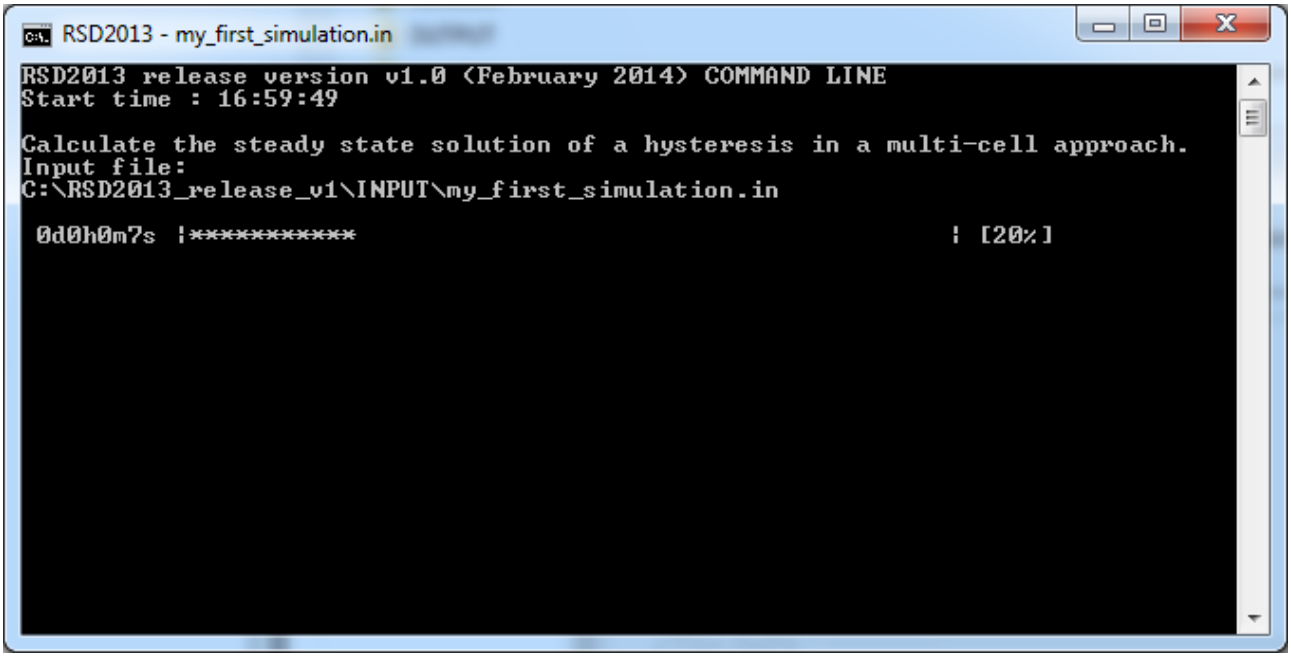
Saving input main file.

The name of the main input file is now listed in the left side window and selected if it is blue highlighted.



List of input files.

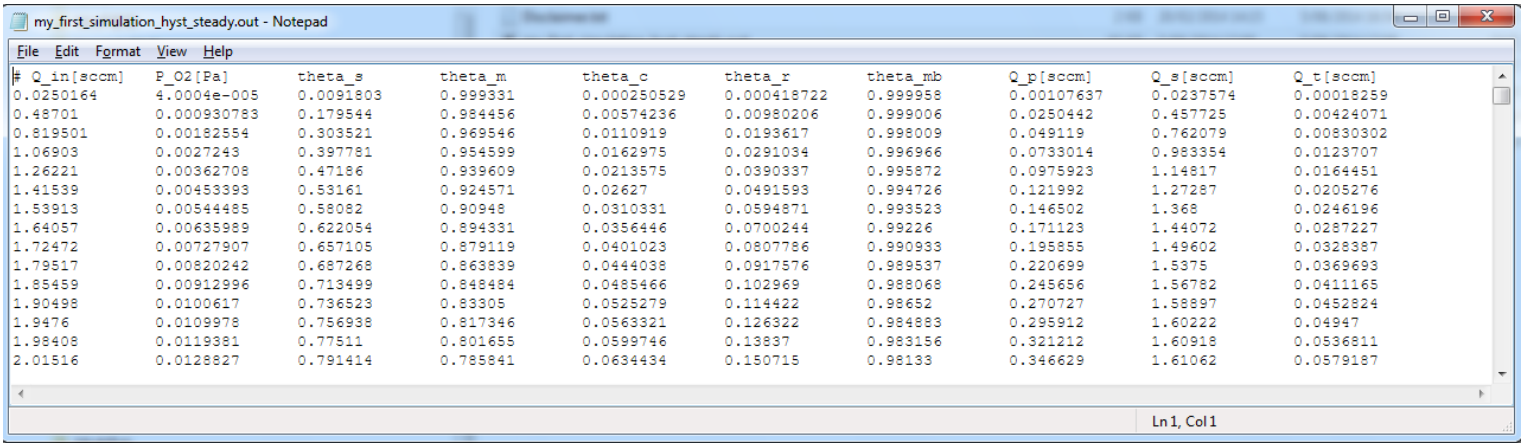
To run the simulation of this selected input file, choose in the menu bar `Simulation` > `Run selected` or press on the icon  . If everything goes well, a command window pops up, showing the progress of the simulation which closes itself on the end of the simulation.



Running simulation.

To look at the simulation results you have to know where the output files are saved. To check this, go to the window tab `Output`. In the first text field next to the button `Choose`, the location where the output files are saved is given. By default the output location is the RSD program folder. The text field underneath gives the prefix string with which every output file will start. By default this string is the name of the main input file. Browsing to the output file location with Windows explorer, you will see two output files recognizable by the extension `.out`. The file ending with `summary.out` is always generated. This file is updated during the simulation run and shows the progress of the simulation as given by the command window. At the end of the simulation it gives the elapsed time for this simulation run and its ending time. The other file ending with `hyst_steady.out` contains the simulation results. As this is a steady state simulation, the reactive gas pressure (second column) is increased up to the value 0.2 as specified in field `Maximum pressure (Pa)` in the window tab `Method`, and subsequently decreased. The total number of pressure values that are calculated, by default 300, is specified by the field `Calculated points` under the same window tab `Method`. The columns of this output file with the steady state solution gives the results of the following variables:

1. Q_in : flow of reactive gas introduced in the vacuum chamber
2. P_O2 : pressure of reactive gas
3. theta_s : spatial averaged compound fraction on substrate surface
4. theta_m : spatial averaged metal fraction on target surface
5. theta_c : spatial averaged chemisorbed fraction on target surface
6. theta_r : spatial averaged compound fraction on target surface
7. theta_mb : spatial averaged metal fraction of target subsurface layer
8. Q_p : reactive gas flow pumped away by the vacuum pump
9. Q_s : reactive gas flow consumed by compound formation on the substrate
10. Q_t : reactive gas flow consumed (or released) by the target


my_first_simulation_hyst_steady.out - Notepad

File Edit Format View Help

# Q_in[sccm]	P_O2[Pa]	theta_s	theta_m	theta_c	theta_r	theta_mb	Q_p[sccm]	Q_s[sccm]	Q_t[sccm]
0.0250164	4.0004e-005	0.0091803	0.999331	0.000250529	0.000418722	0.999958	0.00107637	0.0237574	0.00018259
0.48701	0.000930783	0.179544	0.984456	0.00574236	0.00980206	0.999006	0.0250442	0.457725	0.00424071
0.819501	0.00182554	0.303521	0.969546	0.0110919	0.0193617	0.998009	0.049119	0.762079	0.00830302
1.06903	0.0027243	0.397781	0.954599	0.0162975	0.0291034	0.996966	0.0733014	0.983354	0.0123707
1.26221	0.00362708	0.47186	0.939609	0.0213575	0.0390337	0.995872	0.0975923	1.14817	0.0164451
1.41539	0.00453393	0.53161	0.924571	0.02627	0.0491593	0.994726	0.121992	1.27287	0.0205276
1.53913	0.00544485	0.58082	0.90948	0.0310331	0.0594871	0.993523	0.146502	1.368	0.0246196
1.64057	0.00635989	0.622054	0.894331	0.0356446	0.0700244	0.99226	0.171123	1.44072	0.0287227
1.72472	0.00727907	0.657105	0.879119	0.0401023	0.0807786	0.990933	0.195855	1.49602	0.0328387
1.79517	0.00820242	0.687268	0.863839	0.0444038	0.0917576	0.989537	0.220699	1.5375	0.0369693
1.85459	0.00912996	0.713499	0.848484	0.0485466	0.102969	0.988068	0.245656	1.56782	0.0411165
1.90498	0.0100617	0.736523	0.83305	0.0525279	0.114422	0.98652	0.270727	1.58897	0.0452824
1.9476	0.0109978	0.756938	0.817346	0.0563321	0.126322	0.984883	0.295912	1.60222	0.04947
1.98408	0.0119381	0.77511	0.801655	0.0599746	0.13837	0.983156	0.321212	1.60918	0.0536811
2.01516	0.0128827	0.791414	0.785841	0.0634434	0.150715	0.98133	0.346629	1.61062	0.0579187

Ln 1, Col 1

Example of output file.

Graphical User Interface (GUI)

The graphical user interface (GUI) is designed to create input files for a RSD simulation in an user-friendly way. These input files can also be manually composed. Single or multiple simulation(s) can also be executed from within the GUI. The GUI can be accessed by the executable `RSD2013_GUI.exe`. It most important task is to compose the input files for the simulation executable `RSD2013.exe`. In fact, when starting a simulation from within the GUI, it opens a command line and runs the `RSD2013.exe` executable with as single argument the path of the main input file.

Concept

The concept of the GUI is doing the following tasks:

- create new input files
- load existing input files
- edit input files
- run single or multiple simulations
- setup a series of simulations (see Scan)

In obtaining this, the philosophy of the GUI is as follows. The input of a single simulation is defined in the

window tabs, namely `Method`, `Chamber`, `Target`, `Substrate` and `Output`. The window at the left of the window tabs lists the different simulations. Existing input files can be loaded or new input files can be created. The name within the list is the name of the main input file of a particular simulation. After selecting one or more items in the list, the user can let sequentially run these simulations.

Menu

The menu bar is located at the top of the GUI window. Through this menu the user can

- open or load existing simulations (see File)
- create new simulations (see File)
- save changes to simulations (see File)
- start simulations (see Simulation)
- abort running simulations (see Simulation)

The action of every menu item is explained below.

File

Open

To open or load an existing main input file for editing. Made changes will be saved to the original main input file and their included input files.

Hotkey: Ctrl+O

Open as copy

To open or load a copy of an existing main input file for editing. A new name and saving location is asked for the copy. Changes are saved to the created copy. Only the main input file is copied which contains links to the original included input files. Made changes to these included input files will as such be saved to the originals.

New

To internally open a new input item. It resets the fields in the window tabs to their default values. The input is unsaved (and unlisted) until the `Save` or `Save as ...` item or icon is used.

Hotkey: Ctrl+N

Save

To save the changes made in the window tabs to the main and included input files. The made changes in the window tabs are saved to the current selected (blue highlighted) item in the window list. If no main input file is assigned yet, this action corresponds to a `Save as ...` action.

Selecting an other item in the window list, which is loaded into the window tabs, initiates this `Save` action for the previous selected item.

Hotkey: Ctrl+S

Save as ...

To save and specify a new main input file for the current input of the window tabs. A new main input file is generated together with the included input files. The main input file is added to the list of simulation inputs.

Exit

To exit and close the GUI window.

Simulation

Run selected

To execute the selected (blue highlighted) items of the window list in sequence.

Hotkey: Ctrl+R

Run all

To execute all the items of the window list in sequence, independent if they are selected or not.

Auto prefix

When ticked on, it will replace the value of the field `Prefix for output files:` in the window tab `Output` of all items in the window list by a three digit number in the same order as the are listed. Numbering starts from 000.

Remark: When two or more items in the window list have the same prefix for the output files, a warning will appear. In this case, simulation results will overwrite each other.

Kill current run

To kill or abort all running RSD simulations. In fact, it will kill all running `RSD2013.exe` processes on your platform.

Hotkey: Ctrl+K

Help

About

To show information about the RSD2013 software and to whom it acknowledges.

Menu icons

The menu icons are a selection of common used menu actions. As such their functionality corresponds to a particular menu action.

Open 

See Open.

New 

See New.

Save 

See Save.

Save as 

See Save as ....

Run selected 

See Run selected.

Kill current run

See Kill current run.

About

See About.

Tabs

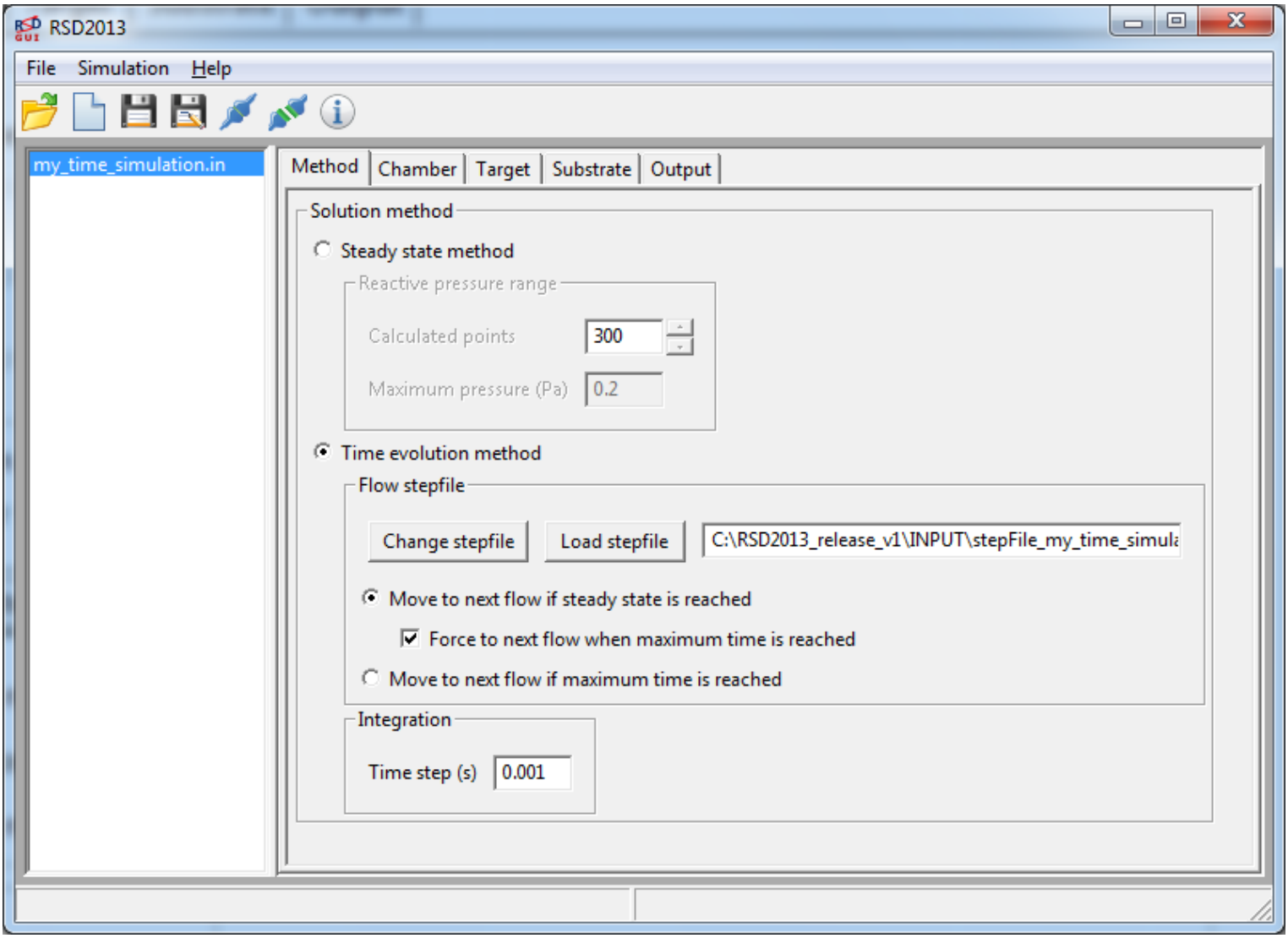
The window tabs graphically represent the information contained in the input files of a selected (blue highlighted) item of the window list. Editing the fields of these tabs changes the simulation input and options.

All simulation options are visual within the window tabs. None used or relevant options or fields are grayed out and unaccessible. They become (un)accessible depending on which simulation choices you make. For example, when choosing the `Steady state method` in the window tab `Method` as solution method, then the fields connected to the `Time evolution method` are irrelevant and as such grayed out.

Most fields have a restricted range of values that can be set. This restriction only applies to the GUI and can be easily overruled by manually editing the input files.

Method

The window tab `Method` basically specifies how the RSD2013 model should be solved. As solution method, two option are available the `Steady state method` and the `Time evolution method`. The choice between the two methods is evidently exclusive.



Method window tab.

Steady state method

To solve the RSD2013 model in its steady state description. The reactive pressure P_r is stepwise increased up to the `Maximum pressure` and subsequently decreased. The total number of reactive pressure P_r values that are calculated are given by the field `Calculated points`.

Calculated points

To define the total number *N* of reactive pressure P_r values that are calculated in the `Steady state method`. So the *N/2* reactive pressure P_r values are each calculated twice, as they can be multi-valued. The first time for an increasing reactive flow Q_{in} and the second time for a decreasing reactive flow Q_{in}.

Maximum pressure

To define the maximal reactive pressure P_r that is calculated in the `Steady state method`.

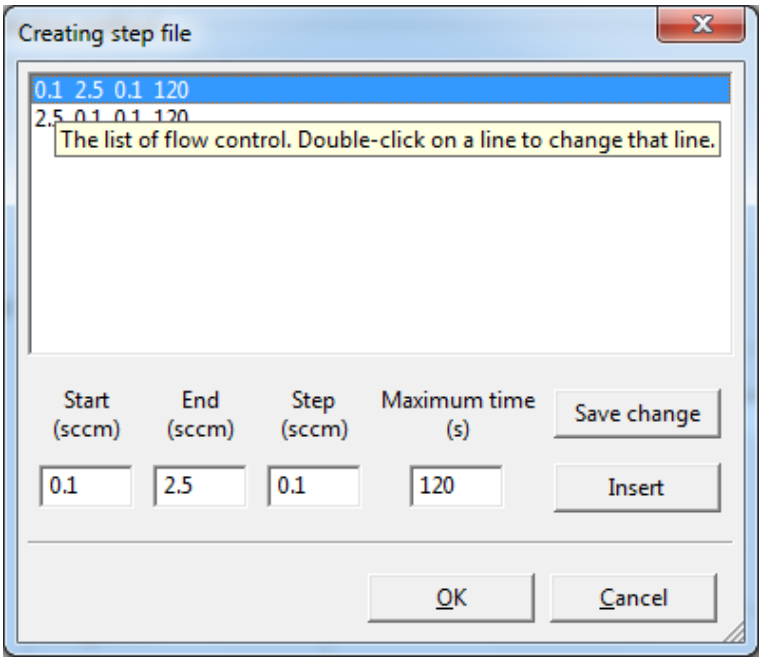
Time evolution method

To solve the RSD2013 model in its time description. The reactive sputter system is evolved in time defined by a given reactive flow Q_{in}. The time evolution of these reactive flows Q_{in} is defined by the so called step file, which is an included input file.

Flow stepfile

The step file is an included input file and defines the evolution of the reactive flow Q_{in} for the time evolution method.

The button `New stepfile` opens the window `Creating step file` where a new step file can be composed.



Creating step file window.

A step file consist out of numerical text lines. The first entry of such line defines the `Start` flow, the second entry the `End` flow, the third entry the `Step` flow with which the `Start` flow is stepwise increased until it reaches the `End` flow. The last entry is the `Maximum time` a given flow is set during a simulation. The `Insert` button adds a line to the step file. The already defined lines are shown as a list in the upper window. By clicking on a line in this list, the line is selected (blue highlighted). By pressing `Del` on the keyboard, you can remove the line. By double clicking, the line is selected and loaded in the editing fields. After making changes

to the line, you can press the `Save change` button to save the changes to the original line. Pressing the `Ok` button pops up a window to specify a saving location and to name the step file. A default name is suggested. It is a concatenation of the string `stepFile` with the name of the main input file. Pressing the `Open` button saves it to the step file.

The button `New stepfile` changes to `Change stepfile` when the full path of an existing step file is specified in the text field. This can be done by direct editing this field or by using the `Load stepfile` button.

Pressing the `Change stepfile` shows the loaded step file in the window `Creating step file` for editing.

Two exclusive options define how the evolution of the reactive flow Q_{in} is handled based on the step file.

- `Move to next flow if steady state is reached` to set the next flow, based on the step file, when a steady state of the system is reached.
    - `Force to next flow if maximum time is reached` to set the next flow, based on the step file, when a steady state of the system is reached OR when the maximum time of the previous flow is elapsed.
- `Move to next flow if maximum time is reached` to set the next flow, based on the step file, when the maximum time of the previous flow is elapsed.

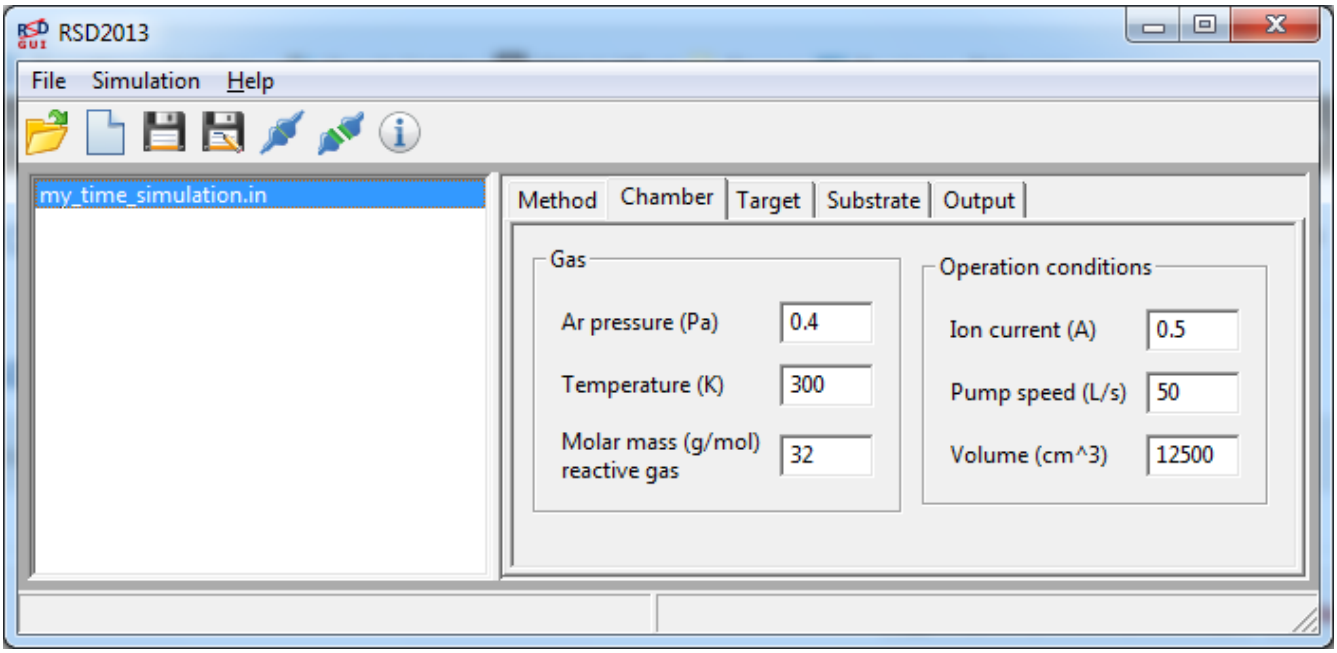
Integration

Time step

To define the integration step Δt of the explicit 4^{th} order Runge-Kutta integrator of the ordinary differential equations for the variables θ_m, θ_c, θ_r, θ_s and P_r.

Chamber

The window tab `Chamber` specifies the parameters connected to the gases in the chamber and the operation conditions.



Chamber window tab.

Ar pressure

To define the fixed pressure P_i of the inert argon gas in the vacuum chamber.

Units : Pa

Temperature

To define the temperature T of the gases.

Units : K

Molar mass reactive gas

To define the molar mass of the reactive gas molecules.

Units : g mol^{-1}

Ion current

To define the total ion current I_{tot} towards the target.

Units : A

Pump speed

To define the volumetric pumping speed S of the vacuum system.

Units : L s^{-1}

Volume

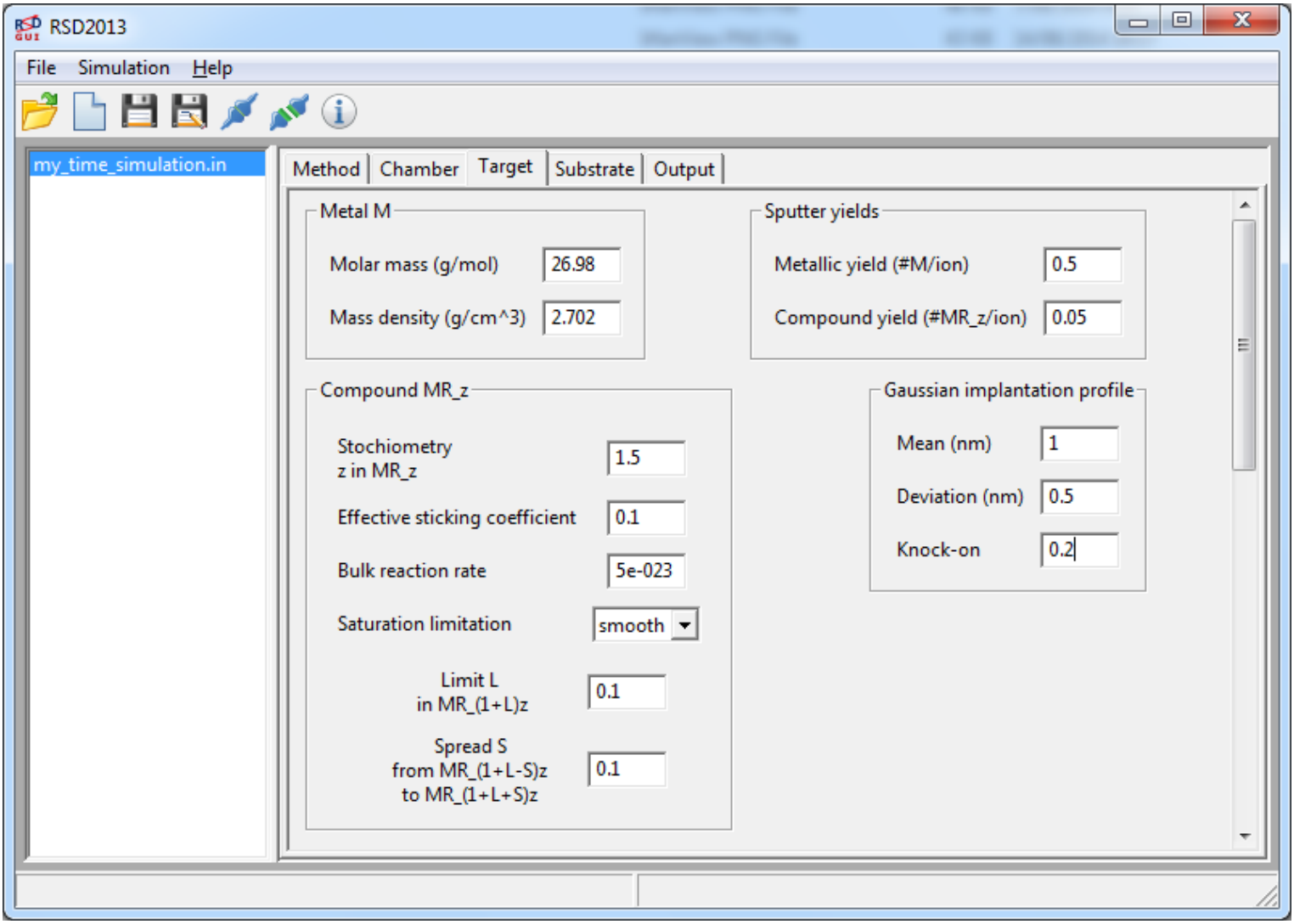
To define the volume V of the vacuum system occupied by the gases. This parameter is grayed out when choosing the `Steady state method`.

Units : m^3

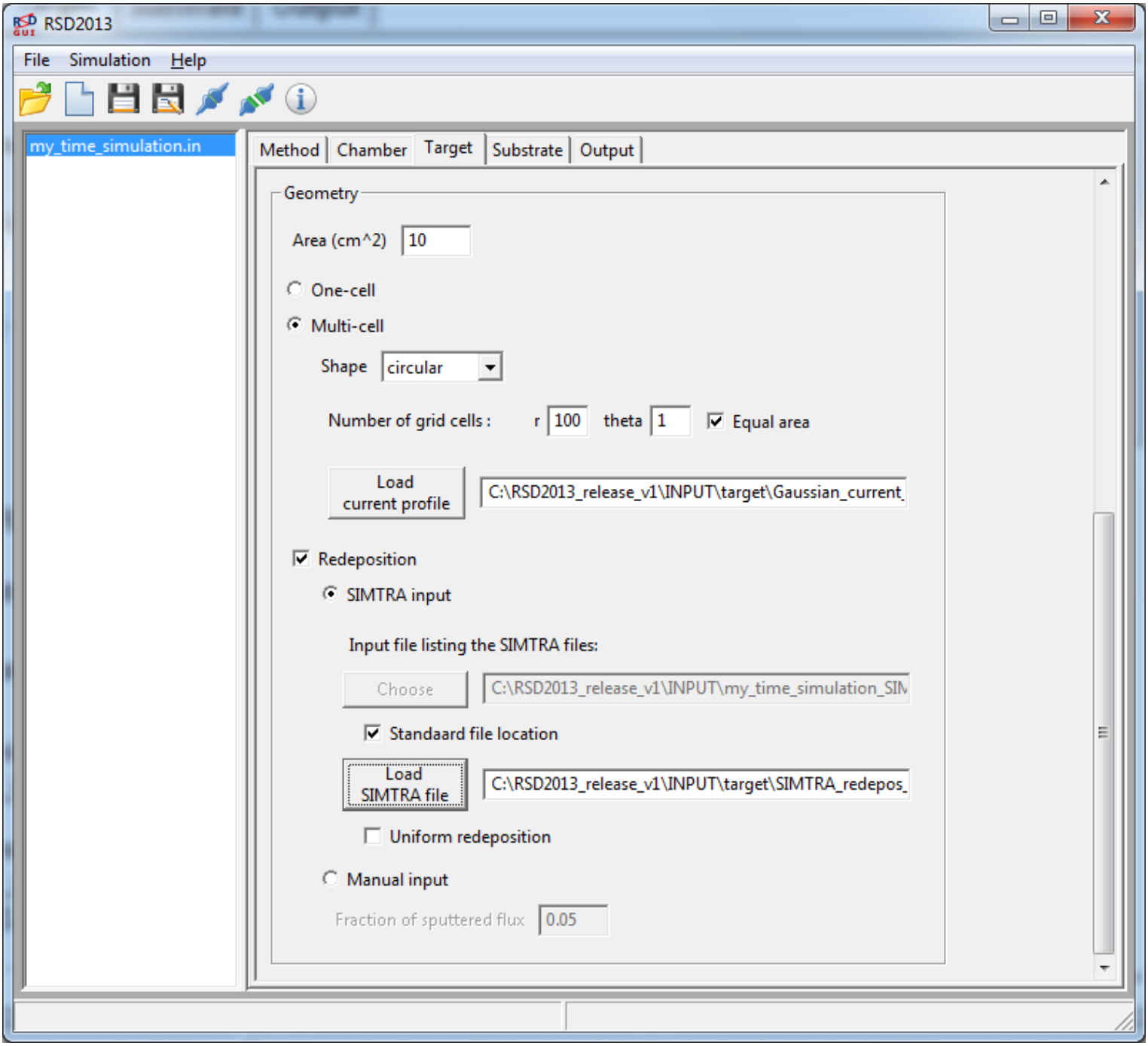
Target

The window tab `Target` specifies the properties connected to the sputtering target. Three additional options are available:

- a saturation limit on the implanted reactive species
- a spatial resolved target by defining a current distribution
- considering deposition on the target (=redeposition)



Target window tab (part 1).



Target window tab (part 2).

Molar mass

To define the molar mass of the metal element that is been sputtered.

Units : g mol^{-1}

Mass density

To define the mass density of the metal in the target. A metal particle density n_0 is calculated from the `Mass density` and the `Molar mass`. This density n_0 is the density of the metal in the target independent if the metal is bound to reactive atoms or unbound.

Units : g cm^{-3}

Metallic yield

To define the yield of metal particles M per incoming ion if the metal is in the metallic state. No distinction is made between inert or reactive incoming ions.

Units : M ion^{-1}

Compound yield

To define the yield of compound particles MR_z per incoming ion if the metal is in the compound state. No distinction is made between inert or reactive incoming ions.

Units : MR_z ion^{-1}

Stoichiometry

To define the stoichiometry *z* of the compound formed on target (and substrate). Compound is described as a compound particle MR_z, with M the metal atom and R the reactive atom.

Effective sticking coefficient

To define the effective sticking coefficient α_t for the target. It is the average probability for a gaseous reactive particle (atom or molecule) to chemisorb on a metallic surface to form a chemisorbed particle.

Bulk reaction rate

To define the reation rate *k* with which reactive implanted atoms react with metal atoms still in the metallic state to form compound particles.

Units : cm^3 s^{-1} M(R)$_z$

Saturation limitation

To optionally define a saturation limit for the amount of reactive species in the target. This saturation is represented by the saturation function $s(n_M,n_R)$ (= error function) which limits the amount of reactive atoms that get implanted. The three choices are:

- `none` no saturation limit ($n_{R,max}=\infty$)
- `abrupt` $s(n_M,n_R)$ is a step function ($\Delta n_R=0$)
- `smooth` smooth growing limit ($\Delta n_R>0$)

In the case of an `abrupt` and `smooth` saturation, a `Limit L` has to be specified. This limit *L* defines the allowed over or under stoichiometry according to the formula $MR_{(1+L)z}$. This limit encloses as well the bounded as unbounded reactive atoms.

For the case of a `smooth` saturation, an additional `Spread S` has to be specified. This spread *S* determines how 'fast' a complete saturation is established. The limitation starts from $MR_{(1+L-S)z}$ to a full saturation at $MR_{(1+L+S)z}$.

Mean

To define the mean R_p of the Gaussian distribution with which reactive ions or knocked on reactive atom gets implanted into the target.

Units : nm

Deviation

To define the deviation dR_p of the Gaussian distribution with which reactive ions or knocked on reactive atoms

get implanted into the target.

Units : nm

Knock-on

To define the knock-on yield &beta. This is the average probability that an incoming ion (inert or reactive) knocks a chemisorbed reactive atom at the surface into the target.

Area

To define the area of the target that is sputtered.

Units : cm^2

One-cell

The `One-cell` choice considers the target as spatial uniform. The ion current density is uniform and the state of the target surface and subsurface is considered homogeneous.

Multi-cell

The `Multi-cell` choice considers the target as spatial resolved in a number of target cells. Two geometrical shapes of the target are selectable `circular` or `rectangular`.

For the `circular` shape the partitioning in the radial dimension `r` has to be specified as well as the partitioning in the azimuthal dimension `theta`. Ticking the `Equal area` box equals the area of each target cell by a non-equidistant partitioning of the radial dimension `r`.

For the `rectangular` shape the partitioning in the horizontal dimension `x` and in the vertical dimension `y` has to be specified. These target cells are automatically equal in area.

With the button `Load current profile` the file location of the included input file current profile has to be given or by direct editing the text box. The current profile file has to correspond with the chosen `Shape`.

Redeposition

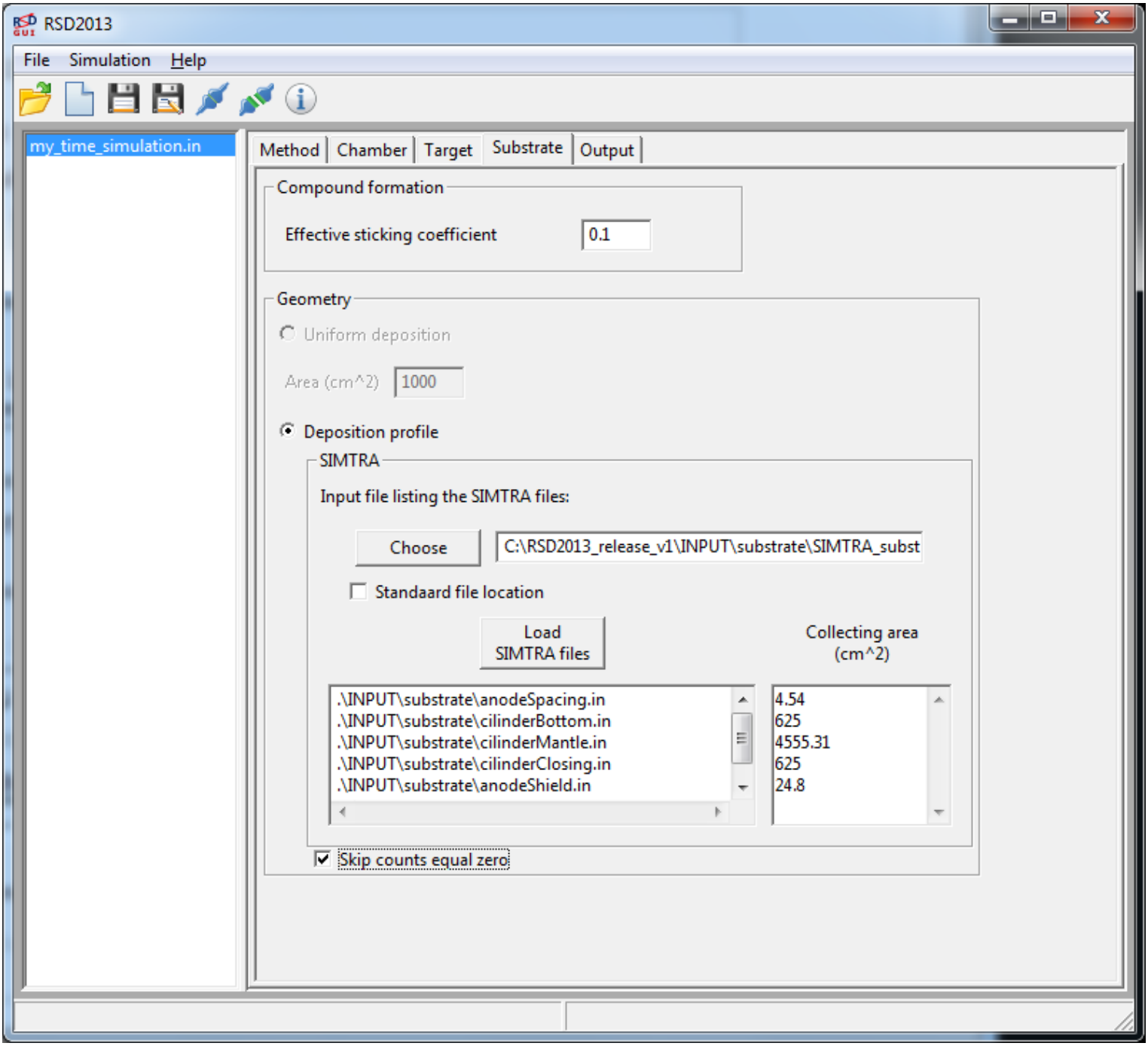
By ticking the `Redeposition` box, the deposition of sputtered material back on the target is considered. Two exclusive ways of defining this redeposition are available: a `SIMTRA input` or a `Manual input`.

For the `SIMTRA input` the deposition profile file for the target has to be provided. This file normally comes from a SIMTRA simulation. With the button `Load SIMTRA file` the file location of the included input file deposition profile has to be given or by direct editing of the text box. This file is added to an included input file listing the deposition profile files of the target. For the moment this SIMTRA listing file will always contain only one entry as only one deposition profile is connected to the target. Ticking the box `Uniform deposition` will calculated based on the deposition profile file, the total fraction of sputtered material that is redeposited. This amount will be equally divided over the target cells.

For the `Manual input` the `Fraction of sputtered flux` has to be defined. This is the total fraction of sputtered material that is redeposited on the target. This fraction will be equally divided over the target cells.

Substrate

The window tab `Substrate` specifies the properties connected to the substrate surfaces. Two exclusive options are available namely `Uniform deposition` and `Deposition profile`.



Substrate window tab.

Effective sticking coefficient

To define the effective sticking coefficient α_s for the substrate. It is the average probability for a gaseous reactive particle (atom or molecule) to chemisorb on a metallic surface to form a chemisorbed particle.

Uniform deposition

The `Uniform deposition` choice considers the substrate as spatial uniform. The deposition distribution is uniform and the state of the substrate surface is considered homogeneous.

Area

When choosing `Uniform deposition`, the total collecting area of the substrate has to be specified

Units: cm^2

Deposition profile

The `Deposition profile` choice considers the substrate as spatial resolved in a number of substrate cells. Deposition profile files have to be provided for this option. This can be done by using the `Load SIMTRA files` button. Multiple deposition profile files can be simultaneously loaded in that way. After clicking open, the file locations are listed in the text field below. The text field `Collecting area` forms the list of the substrate areas that the loaded deposition profiles represent. With each deposition profile file should correspond an area.

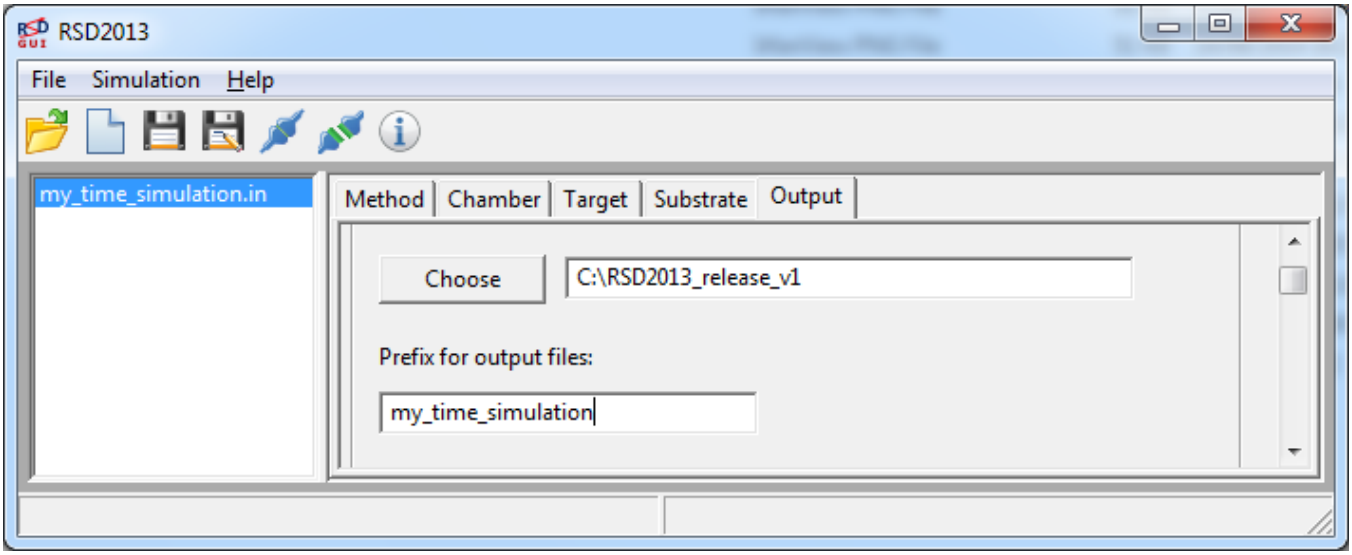
These deposition files are added to an included input file listing the deposition profile files and the corresponding collecting area of the substrate. By default this listing file is saved at its `Standaard file location`. Unticking this box let you specify an other location by either using the `Choose` button or by directly editing the text field next to it. If you choose an existing listing file, the user has the choice to overwrite it or to load the deposition profile files of this listing file.

The `Collecting area` items are in units of cm^2. Their value should always correspond to an area of a rectangle, as the SIMTRA program always represent a surface on a rectangular grid.

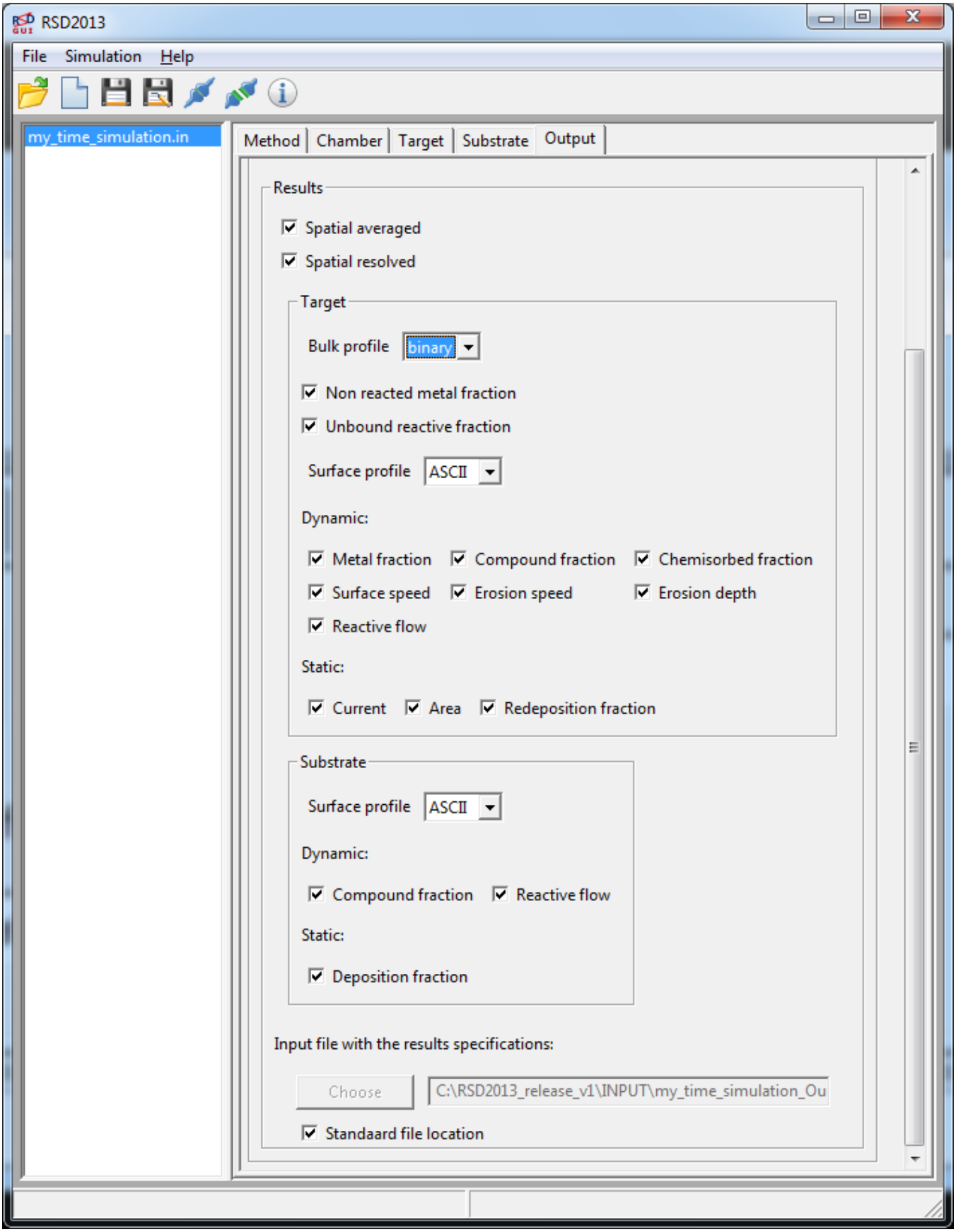
Ticking the box `Skip counts equal zero` will exclude those substrate cells that are assigned a zero deposition fraction. These substrate cells are considered to be not existing, and a value of -1 will appear in the output file for those cells.

Output

The window tab `Output` specifies which results should be printed out and where to save them.



Output window tab (part 1).



Output window tab (part 2).

Output directory

To define the directory where all output files will be placed. This directory can be specified by direct editing of the text field or by using the `Choose` button.

Prefix

To define the prefix string for the file name of all output files. By default this will be the file name of the main input file. Ticking the Simulation>Auto prefix will attribute a number to the prefix field and gray out this field.

Results

By ticking the check boxes, the desired output can be selected. The available outputs, those that are not grayed out, depend on previous choices and selected options. For example, when choosing the One-cell in the Target tab and Uniform deposition in the Substrate tab, only the Spatial averaged check box can be chosen.

Ticking the Spatial averaged check box will create an output file with suffix steady.out in the case of the Steady state method and a second output file with suffix time.out in the case of the Time evolution method. Additional info about these output files can be found in the section Spatial averaged.

Ticking the Spatial resolved check box will be possible when choosing the Multi-cell option in the window tab Target and/or the Deposition profile option in the window tab Substrate. The corresponding check boxes will become available.

Two output formats can be chosen for the spatial resolved data: ASCII or binary. The binary format is much compacter compared to the regular ASCII format. The structure of the numerical data is nevertheless the same, only will every numerical be represented by a 32 bit IEEE float value.

Bulk profile means that 3 dimensional data is generated within a volume, while Surface profile means that 2 dimensional data is generated on a surface.

Following table summarizes the output possibilities:

Check box	Variable	Suffix string	Volume	Surface	Dynamic	Static
Target						
Non reacted metal fraction	n_M/n_0	target_bulk_n_M.out	yes	no	yes	no
Unbound reactive fraction	n_R/n_0	target_bulk_n_f.out	yes	no	yes	no
Metal fraction	θ_m	target_surf_thetaM.out	no	yes	yes	no
Compound fraction	θ_r	target_surf_thetaR.out	no	yes	yes	no
Chemisorbed fraction	θ_c	target_surf_thetaC.out	no	yes	yes	no
Surface speed	v_s	target_surf_surfSpeed.out	no	yes	yes	no
Erosion speed	v_e	target_surf_erosionSpeed.out	no	yes	yes	no
Erosion depth	-	target_surf_erosionDepth.out	no	yes	yes	no
Reactive flow	Q_t	target_surf_Qt.out	no	yes	yes	no
Current	I	target_surf_current.out	no	yes	no	yes
Area	A_t	target_surf_area.out	no	yes	no	yes
Redeposition fraction	ε_t	target_surf_redepos.out	no	yes	no	yes
Substrate						
Compound fraction	θ_s	target_surf_thetaS.out	no	yes	yes	no
Reactive flow	Q_s	target_surf_Qs.out	no	yes	yes	no
Deposition fraction	ε_s	target_surf_depos.out	no	yes	no	yes

The selection of data and the saving format is stored in an included input file. By default this included input file is saved at its Standaard file location. Unticking this box let you specify an other location by either using the Choose button or by directly editing the text field next to it. If you choose an existing input file with output specifications, the user has the choice to overwrite it or to load the output specifications from this file.

List

The window list lists the loaded or created simulation inputs. An item in the list is represented by the filename of the main input file connected to a simulation. By clicking on an item in the list, the simulation input is

loaded into the window tabs for editing.

The simulation input which is current in scope is blue highlighted in the list. Selecting another item in the list will save the made changes in the previous simulation input.

Multiple items in the list can be selected (=blue highlighted) to perform one of the following actions:

- Remove the item from the list by pressing the `Del` key. Note that the input files are NOT removed from your disk, only from the list.
- Run the simulation by pressing `Simulation>Run selected` in the menu bar or the menu icon.

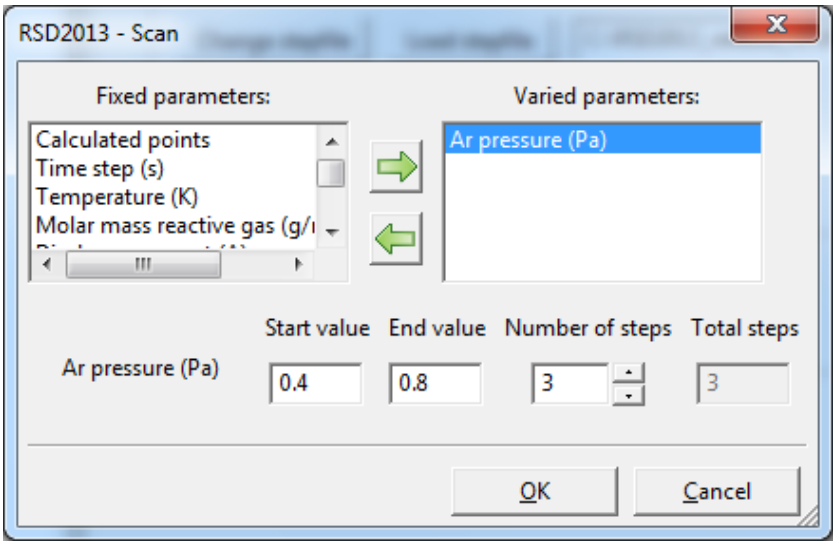
Right-clicking with the mouse on a selected (=blue highlighted) item in the list shows the following actions:

- `Scan`

Scan

The `Scan` action allows to do a parameter scan. This action is executed on a selected simulation input from the window list. A limited number of parameters of this simulation input can then be varied. For each parameter combination, a new simulation input will be generated and as such be inserted as a new item in the window list.

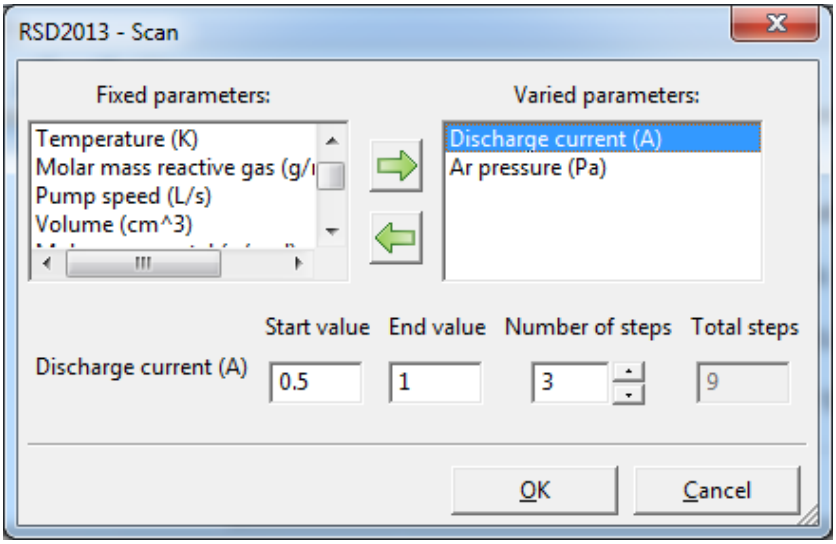
Selecting this `Scan` action for an item in the window list pops up the scan window. Two lists are defined: `Fixed parameters` and `Varied parameters`. The `Varied parameters` list is initial empty. Items of the `Fixed parameters` list can be placed in the `Varied parameters` list by the right arrow and put back by the left arrow.



Scan window, one varied parameter.

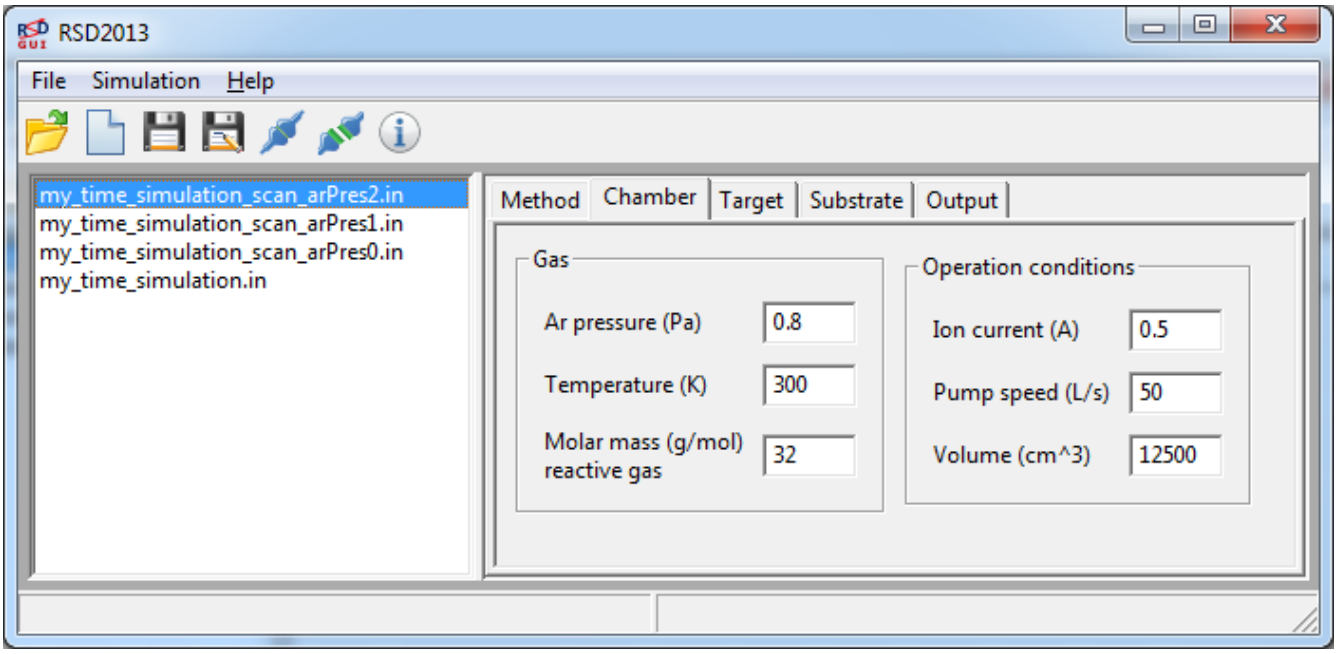
Selecting an item in the `Varied parameters` list let you define a value range over which this parameter should be varied at the bottom of the window. `Start value` sets the lower limit of this range, while `End value` sets the upper limit. `Number of steps` sets the number of parameter values over this range. The lower and upper limit should be counted in.

Multiple items in the `Varied parameters` list results in combined parameters sets. For example, if you have two items in the `Varied parameters` list, each with a `Number of steps` of 3, then 9 (= 3 x 3) simulation inputs will be generated. The total simulation inputs that will be generated, is showed in the non-editable `Total steps` field.

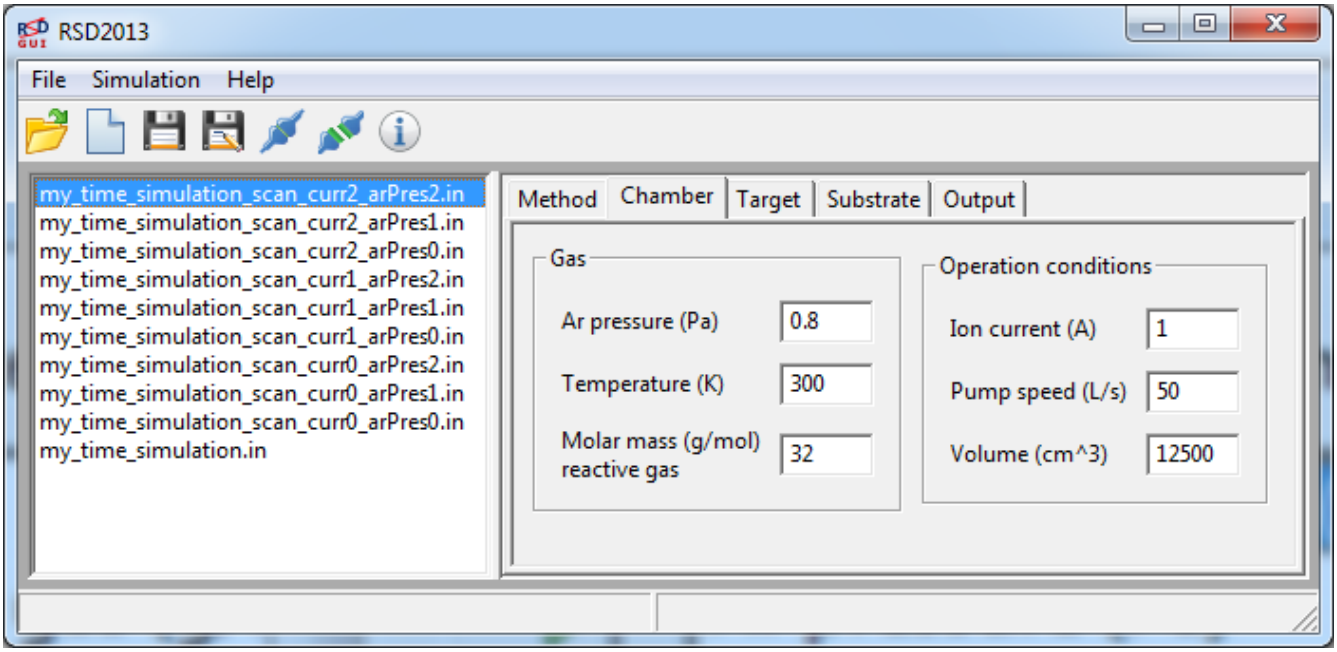


Scan window, two varied parameter.

Pressing `Ok` will generate the simulation inputs and add them to the window list. The file names of the main input file of each item is automatically assigned. The filename of the original main input file is concatenated with the string `scan`, a keyword characteristic for the varied parameter and a number starting from 0 to count the variations. Note that all generated simulation inputs will share the same included input files.



Window list with one varied parameter.



Window list with two varied parameter.

Command line

The RSD2013 simulation software can be used without the GUI. The executable `RSD2013.exe` can directly be executed on a command line if provided with a valid single argument. This argument is the absolute path of a main input file or the relative path with respect to the program directory (where the `RSD2013.exe` executable is located). This is useful if you want to run the RSD2013 simulation in a script.

This main input file and the included input files where it references to, can manually be edited or be created by the GUI.

Input files

The input files define all the input needed for a successful RSD2013 simulation. Two types of input files are distinguished:

- A main input file which contains input parameters, simulation options and path references to the included input files.
- The included input files define more specific input data and options for a simulation or further path references to included input files.

Some input files are allowed to start or contain comment lines. Those file usually begin with an explanation of the structure of that input file. A comment line always starts with `#`.

Main

The main input file is the input file which is provided to the simulation executable `RSD2013.exe`. It contains all data and references to data needed for running the simulation. It is a text based file.

The structure of the file is as follows. Every line starting with `#` is considered a comment line and is ignored. Every other line defines input and starts with the keyword `rowXXX`, where XXX is a number. This keyword `rowXXX` is omitted when reading in the file. Nevertheless, the line number of each text line defines which kind of parameter, option or reference should be defined. Explanation of which kind of information is expected on each line is given in the comment lines starting this file.

As input restrictions are only checked within the GUI, their will no be any validity check of the give input data.

Some additional simulation options can be available which are not (yet) included in the GUI.

Included

The included input files are all other input files then the main input file. The main input file contains references to these included input files, but included input files can also contain further references to other included input files.

A description of the included input files that RSD2013 makes us of is given below.

Step

The step file defines the evolution of the reactive flow Q_{in} for the time evolution method.

This input file can be edited or loaded in the window tab `Method`>`Flow stepfile` when choosing the `Time evolution method`.

The step file is a text based file which consist out of numerical text lines. Each line defines a range over which the reactive flow is varied. The first entry of such a line defines the start flow, the second entry the end flow, the third entry the step with which the start flow is stepwise increased until it reaches the end flow. The last entry is the maximum time a given flow is set, depending on the chosen option for the evolution of the reactive flow.

The first none comment line should contain the number of flow ranges (or numerical text lines) that are specified. The comment lines starting the file explain the structure of this file.

Current profile

The input file with the current profile defines how the total ion current is distributed over the target. Two types of current profile are possible depending on the shape of the target: a circular or a rectangular target.

The current profile file is a text based file. The first non comment line is the keyword `circular` or `rectangular` that can be enclosed by comment lines. The numerical text lines define the profile. The profile should not be necessarily normalized.

For the `circular` case, only an one dimensional radial profile is considered. The first entry of each line is the radial distance, the second entry is the value of the profile at that position. The radial distance is rescale to the target size.

For the `rectangular` case, a two dimensional rectangular profile is considered. The profile is defined on a matrix. The number of columns corresponds with the partitioning of the target in the y dimension while the number of rows with the partitioning in the x dimension. Each element of the matrix corresponds to the value of the profile.

Deposition profile

The deposition profile files define which fraction of the sputtered material is deposited on which surface area. The files are text based and matrix structured as the output deposition files from the SIMTRA software. The first two entries on the first line define respectively the number of rows and columns. The rest of the line is ignored. All following lines define the matrix.

The deposition profile files connected to the substrate (or the target) are listed and referenced in a separate file. This file is structured as follows. The first non comment line of the file gives the number of included deposition profile files. Each following couple of lines represent a deposition profile with on the first line the full path or relative path to the deposition profile file, while on the second line the area corresponding to the deposition profile. This area should take into account the full rectangular matrix of the profile, also when their are (ignored) zero elements.

Substrate

Several deposition profile can be connected to the substrate. These deposition profile files and their connected areas can be assigned when choosing `Deposition profile` in the window tab `Substrate`.

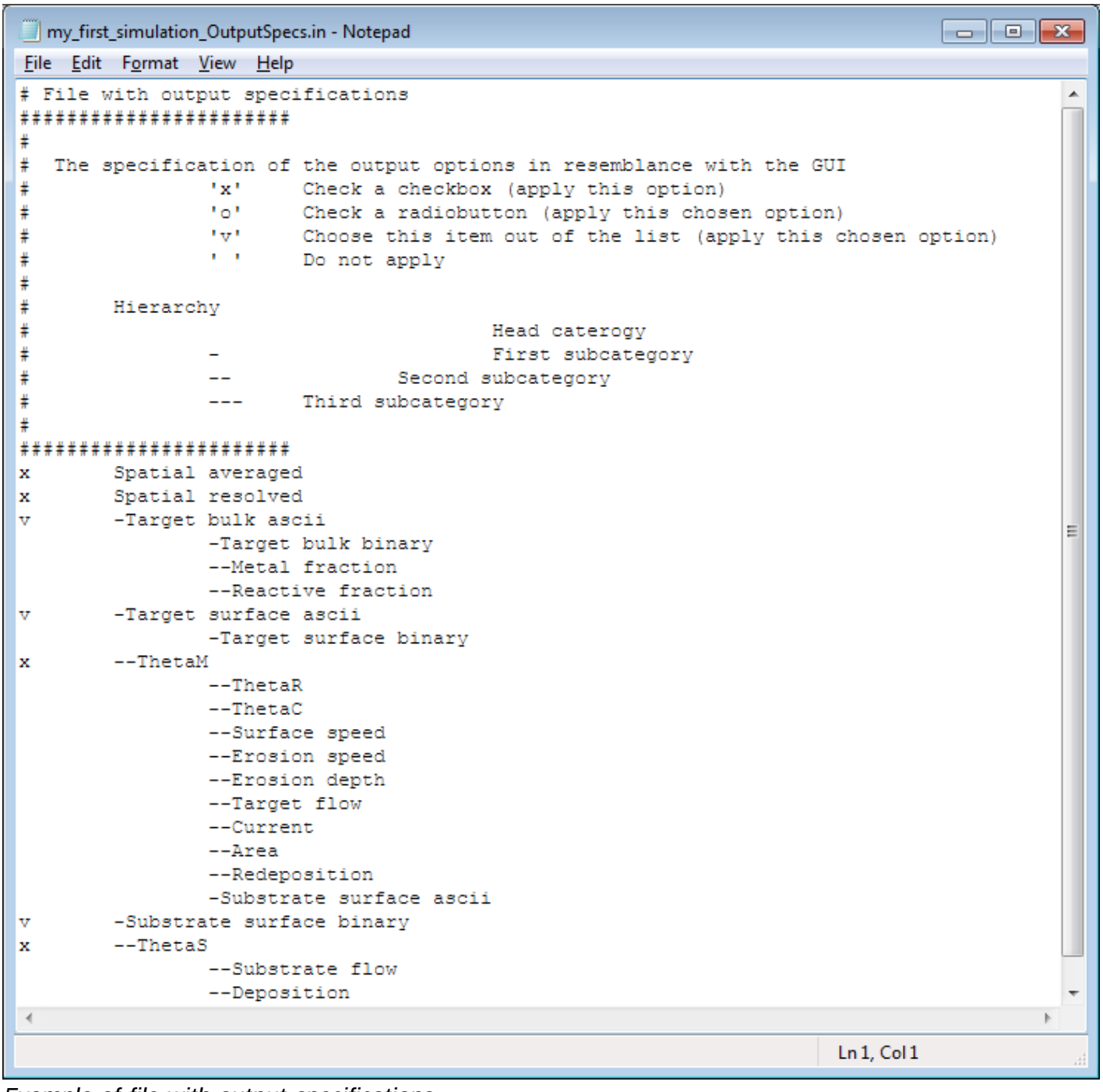
Target

Only one deposition profile can be connected to the target, as only one target is considered for the moment. The deposition profile file can be assigned when choosing `Multi-cell`, `Redeposition` and `SIMTRA input` in the window tab `Target`.

Output specs

The file with the output specifications determines which output will be generated when a simulation is executed. It's appearance is closely related to the window tab `Output`.

To each kind of output is a keyword linked. When this keyword is not preceded by `x`, `o` or `v`, this output is not generated. The `x` is used for a checkbox, the `o` for a radiobutton and `v` for a choice in a roll-down list. An example is given.



Example of file with output specifications.

In this example the spatial averaged variables are generated, the spatial resolved metal fractions on the target are generated in an ASCII format and in binary format the spatial resolved compound fractions on the

substrate are generated.

Output files

Output files always have the extension `.out`. Which output files are produced, is determined by the output specification file or in the window tab `Output`. A summary of the simulation run is always generated and is recognized by the ending string `summary.out`. The file name of each other output file starts with the chosen `Prefix` and ends with an unique string.

Spatial averaged

The output file with the spatial averaged output ends with the string `hyst_steady.out`. For the `Steady state method`, it outputs in each column the following steady state variables

1. Q_in : flow of reactive gas introduced in the vacuum chamber
2. P_O2 : pressure of reactive gas
3. theta_s : spatial averaged compound fraction on substrate surface
4. theta_m : current weighted averaged metal fraction on target surface
5. theta_c : current weighted averaged chemisorbed fraction on target surface
6. theta_r : current weighted averaged compound fraction on target surface
7. theta_mb : current weighted averaged metal fraction of target subsurface layer
8. Q_p : total reactive gas flow pumped away by the vacuum pump
9. Q_s : total reactive gas flow consumed by compound formation on the substrate
10. Q_t : total reactive gas flow consumed (or released) by the target

When choosing for the `Time evolution method`, this file contains the values of the variables at the end of a flow step. Additionally, an extra output file is generated which ends with the string `hyst_time.out`. This file contains the same variables as above, but adds an 11^{th} column with the time elapsed in the simulation.

11. t : time in the simulation

The spatial averaged variables correspond with this time. Every 255 time steps the value of these variables are added to the file.

Spatial resolved

When the target and/or the substrate is spatial resolved by defining respectively a current profile and/or a deposition profile, spatial resolved output can be generated. We consider spatial resolved output on a surface (2D) for the target and the substrate or within a volume (3D) for the target. The format how this data is written to the files can be simple ASCII or in a binary format. In the binary format the structure is the same as for the ASCII format, but every number is binary represented by a 32 bit IEEE float value.

Surface (2D)

Surface resolved output can be generated for the target and for the substrate when choosing a current profile and a deposition profile respectively. A table listing the different variables which can be resolved on a surface is given under `Results`.

The format of the file is as follows. The first entry of the first line of the file is the number of columns which equals the cells in the x or radial dimension. The rest of the first line numbers the columns starting from zero. The first entry on each following line numbers the rows which equals the cells in the y or azimuthal dimension. The following entries on each line represent the variable value in the matrix.

The data on the surface is saved at every steady state point sequentially, restarting the row numbering for each point. A value of -1 means this surface cell is not considered in the simulation. For the different substrate surfaces, the file names are numbered in the same way as they occur in the input file listing the deposition profiles.

Volume (3D)

Volume resolved output can be generated for the target when choosing a current profile. A table listing the different variables which can be resolved within a volume is given under Results.

The format of the file is as follows. The first entry of the first line is 200, the number of columns which equals the in-depth points where a fraction is defined. The rest of the first line defines the depth (in cm) where a variable is resolved. This depth stretches over the implantation zone (which equals $R_p + 3dR_p$ for a Gaussian profile). The first entry on each following line numbers the rows which equals the number of surface cells (product of the number of cells in the y or azimuthal dimension and of the number of cell in the x or radial dimension). The numbering starts with the number of cells in the y or azimuthal dimension for a fixed x or radial cell. The following entries on each line represent the in-depth fractions for the corresponding surface cell.

The data within the volume is saved at every steady state point sequentially, restarting the row numbering for each steady state point.

End remark

The author will be grateful if you make notice of any mistake or typo occurring within this manual. Feel free to contact him at koen.strijckmans@ugent.be.