Documentation of RSD2013v3

(version date 2018/11/29)

Content

Legend

[RSD only] indicates that these parameters/options only apply for the RSD2013 model
`sample text` this text formatting refers that it can be found back on the graphical user interface (GUI) or on your computer
sample text this text formatting refers that it is a link to another section or external source

 indicate possible watch-outs or warnings

 indicate useful hints to setup a simulation

 option is not (yet) available
www link to an external (web)source

Installation

Installation of the RSD2013 software is simple. Unpack the compressed zip file to a location of your choice. You can easily start off using the software by running the `RSD2013_GUI.exe` which opens the graphical user interface (GUI). The RSD2013 software only runs on a Windows platform.

Files and directories

`RSD2013_GUI.exe`

This executable starts the graphical user interface (GUI) of the RSD2013 software. The GUI allows to create the necessary input files and to start up one or more RSD simulations.

`RSD2013.exe`
This executable can only be started from the command line supplied with the main input file. It starts an individual RSD simulation specified by this main input file which may be generated with the GUI or manually. Renaming `RSD2013.exe` will make running simulations through the GUI impossible.
`Changelog.txt`

This document summarizes the new features and bug fixes in each release of RSD2013.

`README.txt`

Short documentation to quick start the use of RSD2013 and the used formatting conventions of the simulation output.

`Disclaimer.txt`

This document contains the DISCLAIMER OF WARRANTIES AND LIMITATION OF LIABILITY.

`icons`

This directory contains the icons and figures used in the GUI. This directory should be left intact.

`templates`

This directory contains headings which are attached to the generated input files. This directory should be left intact.

`simtra_v2.2` (optional)

This directory contains the Monte Carlo simulation program SiMTra which may be used to produce (re)deposition profile files of the sputtered material on the substrate (and target) surfaces.

`INPUT` (optional)

This directory contains example (main) input files for RSD simulations. It can optionally been used to store your own input files.

`OUTPUT` (optional)

In this directory, the output files from the example RSD simulations be saved. It can optionally been used to save your own simulation output.

Overview

The RSD2013 software is developed to simulate the reactive sputter process of a constant or pulsed DC magnetron. Process operation curves as function of a single `Varied operation parameter` are reproduced where the focus is on a possible hysteresis in the observables as function of this `Varied operation parameter`. Two models are provided: the “original” `Berg` model or the `RSD2013` model. The mathematical formulation of both models can be found in the thesis “Modeling the reactive magnetron sputtering process”www and in the article “ A time-dependent model for reactive sputter deposition”www.

Their can be some confusion in terminology but context should make things clear:
- RSD simulation = simulation with the `Berg` model or the `RSD2013` model
- RSD2013 = either the simulation software as a whole or the specific `RSD2013` model
- RSD input files = input files for a RSD simulation

The following variables are resolved, depending on the used model and the chosen options:

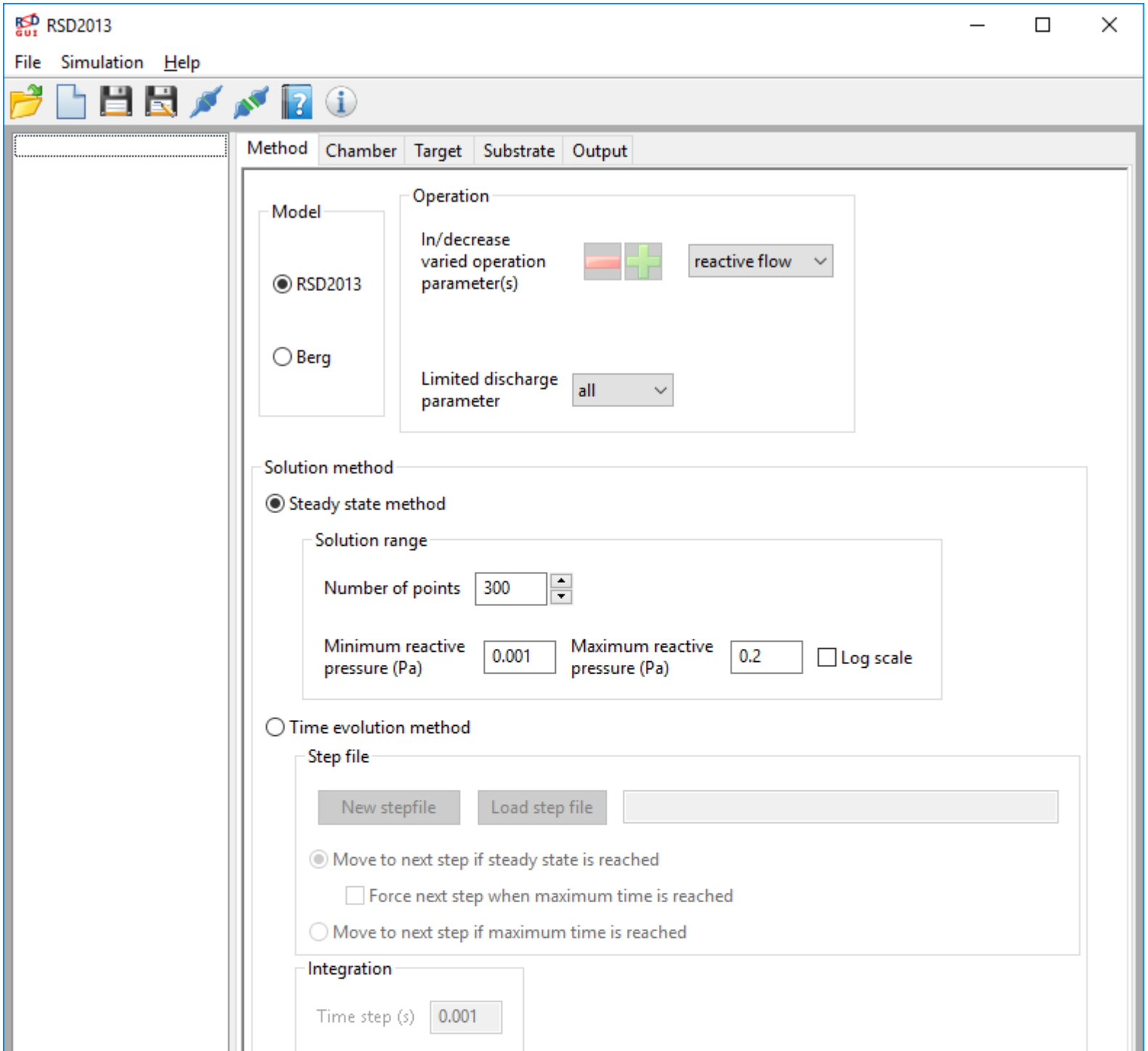
Variable	Units	Description	
p_r	Pa	pressure reactive gas in the system	
θ_m	-	fraction non-reacted metal sites at target surface	
$\theta_{m,ss}$	-	fraction non-reacted metal sites at target surface/subsurface interface	**[RSD only]**

Variable	Units	Description	
θ_c	-	fraction chemisorbed metal sites at target surface	
θ_r	-	fraction reacted metal sites at target surface	**[RSD only]**
θ_s	-	fraction reacted metal sites at substrate surface	
n_M	#M cm^{-3}	concentration non-reacted metal M in target subsurface	**[RSD only]**
n_R	#R cm^{-3}	concentration non-reacted implanted reactive gas atoms R in target subsurface	**[RSD only]**
v_s	cm s^{-1}	surface speed of target	
v_e	cm s^{-1}	erosion speed of target	
d_e	cm	erosion depth of target	
ε_t	cm^{-2}	redeposition fraction surface density	**[RSD only]**
ε_s	cm^{-2}	deposition fraction surface density	
Q_r	sccm	flow of molecular reactive gas introduced into the vacuum chamber	
Q_t	sccm	flow of molecular reactive gas initially getterd by the target	
Q_s	sccm	flow of molecular reactive gas gettered by the substrates	
Q_p	sccm	flow of molecular reactive gas gettered by the vacuum pump	
S	Ls^{-1}	pumping speed by the vacuum pump	
I	A	discharge current	
I_{ion}	A	discharge ion current	
V	V	discharge voltage	

These variables are resolved by the models on the condition that several material and operation parameters are specified as input. These input parameters are clarified throughout the following sections.

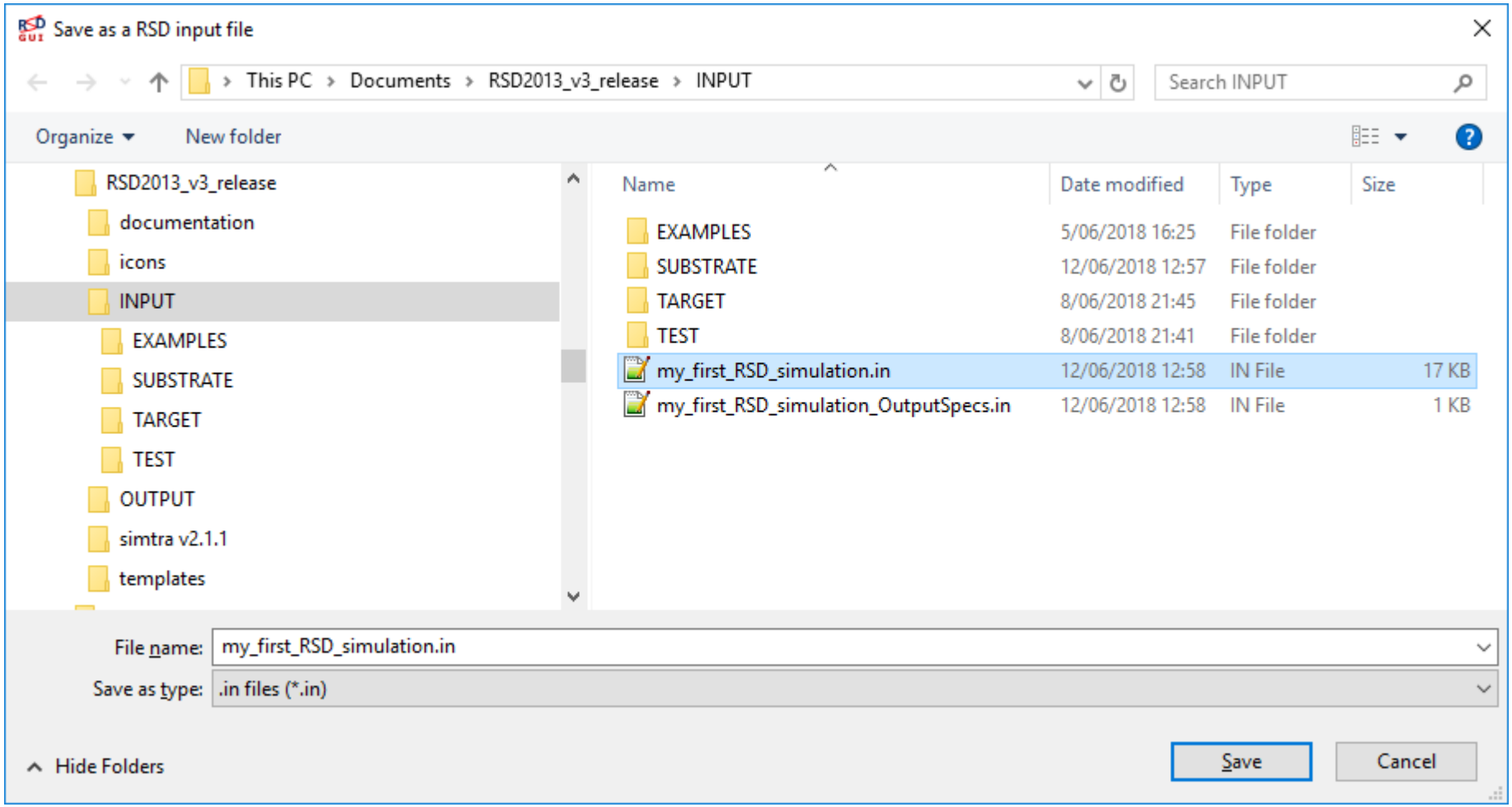
Quick start

To run a first 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`.


RSD2013
File
Simulation
Help
Method
Chamber
Target
Substrate
Output
Model
RSD2013
Berg
Operation
In/decrease varied operation parameter(s)
reactive flow
Limited discharge parameter
all
Solution method
Steady state method
Solution range
Number of points
300
Minimum reactive pressure (Pa)
0.001
Maximum reactive pressure (Pa)
0.2
Log scale
Time evolution method
Step file
New stepfile
Load step file
Move to next step if steady state is reached
Force next step when maximum time is reached
Move to next step if maximum time is reached
Integration
Time step (s)
0.001

Default input.

To run this default simulation, save first the simulation input. By choosing `File` > `Save as ...` in the menu bar or  , 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_RSD_simulation.in`. Press the `Save` button. Two input files will be created, namely `my_first_RSD_simulation.in` and `my_first_RSD_simulation_OutputSpecs.in`. The first file is the main input file, while the second file is the results specification file. These specifications are defined in the window tab `Output` under `Results`.

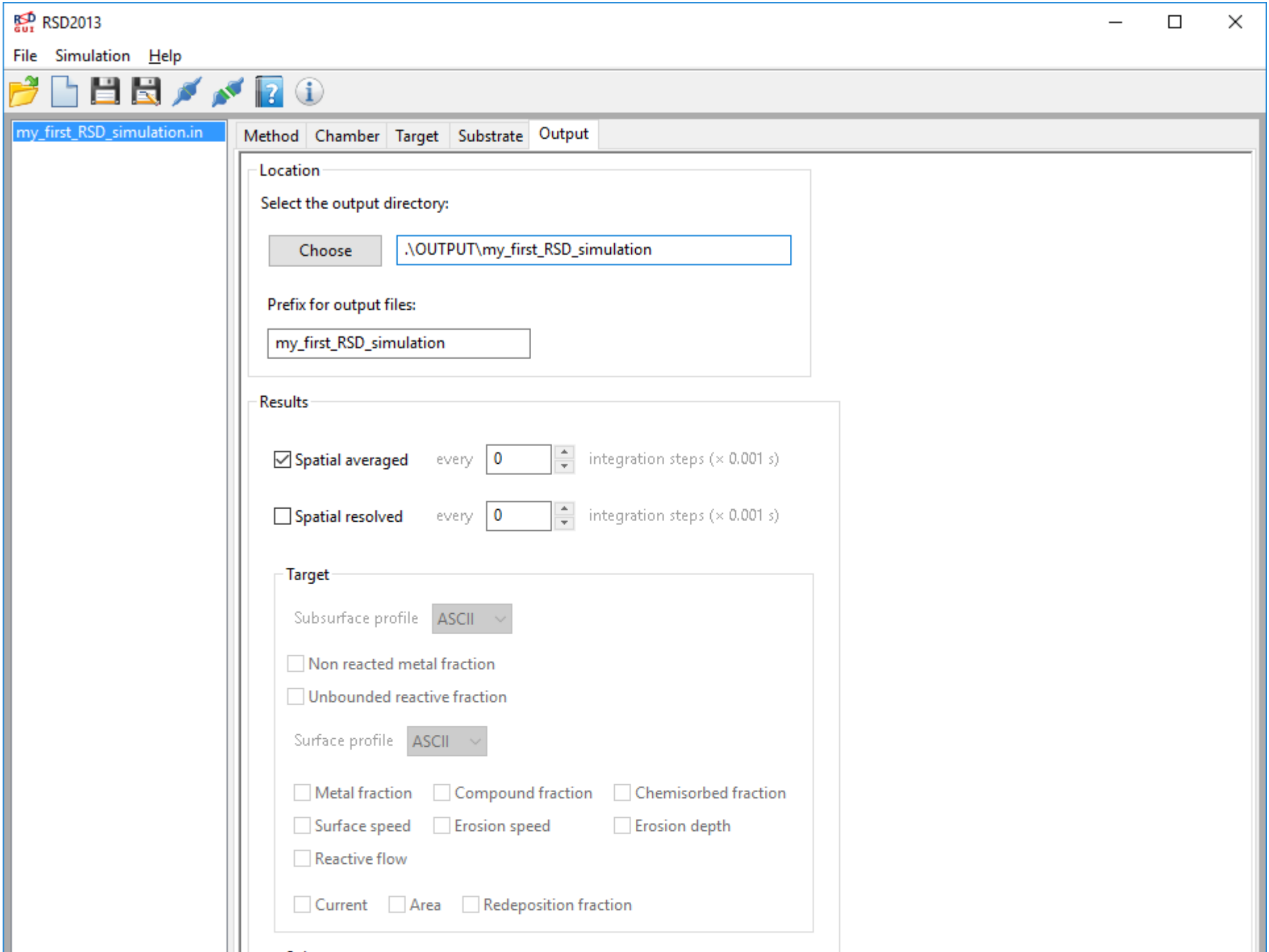


Saving input main file.

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

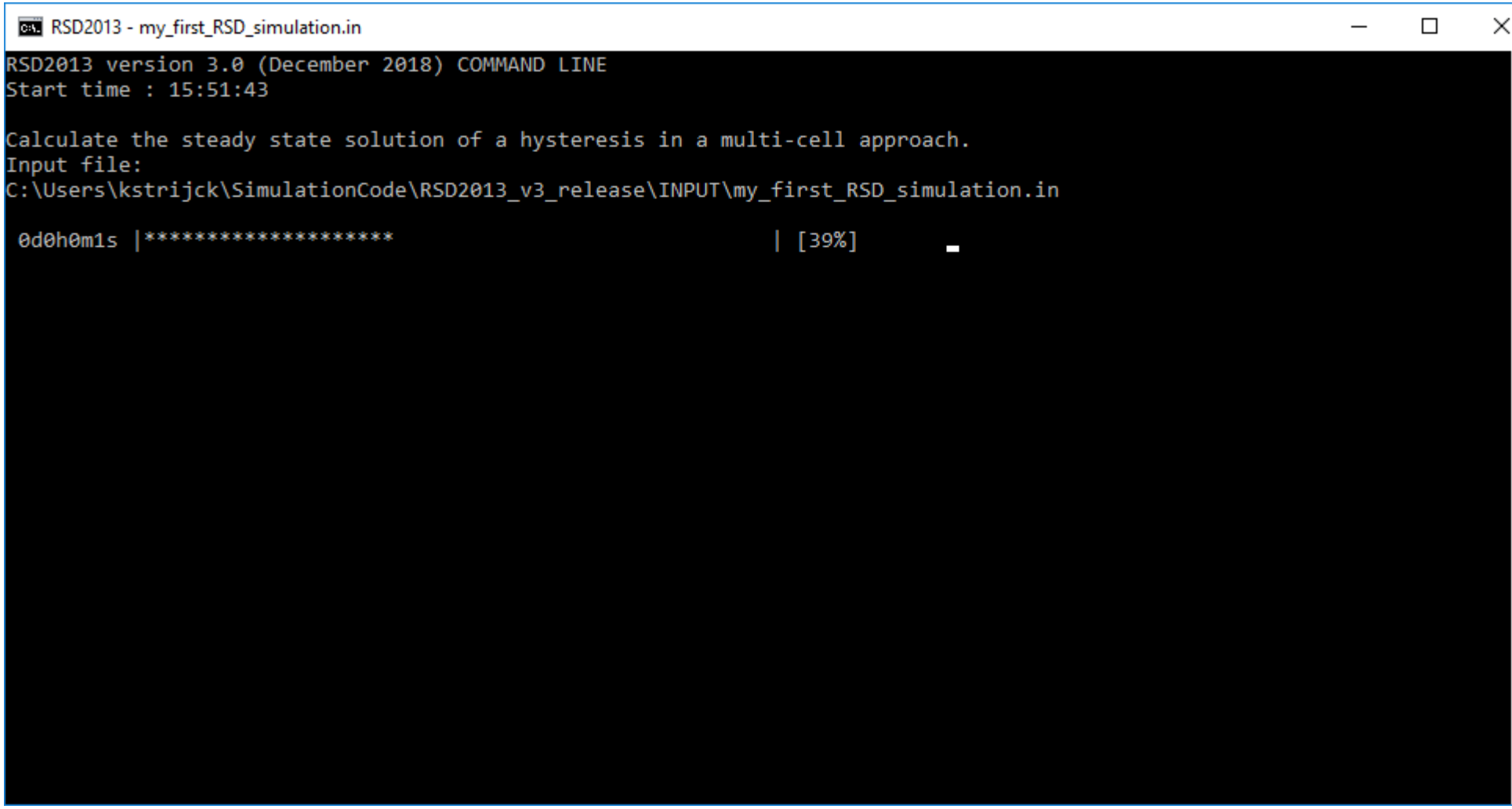
On the first saving of the input file or using `File` > `Save as ...`, the `Select the output directory:` and the `Prefix for output files:` will be automaticly (re)assigned based on the file name. A new output directory with the file name as name is created, one level up

in the directory tree that was specified in `Select the output directory:`. We changed this output directory to `.\OUTPUT\my_first_RSD_simulation` which will save the output to the relative directory within the program directory.


RSD2013
File
Simulation
Help
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Location
Select the output directory:
Choose
.\OUTPUT\my_first_RSD_simulation
Prefix for output files:
my_first_RSD_simulation
Results
Spatial averaged
every
0
integration steps (× 0.001 s)
Spatial resolved
every
0
integration steps (× 0.001 s)
Target
Subsurface profile
ASCII
Non reacted metal fraction
Unbounded reactive fraction
Surface profile
ASCII
Metal fraction
Compound fraction
Chemisorbed fraction
Surface speed
Erosion speed
Erosion depth
Reactive flow
Current
Area
Redeposition fraction

List of input files.

To run the simulation of this selected input file, choose in the menu bar `Simulation` > `Run selected` or  . If everything goes well, a command prompt 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 field `Select the output directory:` next to the button `Choose`, the location where the output files are saved is given. The field `Prefix for output files:` underneath gives the prefix string which every output file will start with. By default this string is the name of the main input file. When browsing to the output file location with Windows explorer, you will see two output files recognizable by the extension `.out` and two log files recognizable by the extension `.log`. 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 prompt 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 reactive 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 `Number of 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_r : flow of reactive gas introduced in the vacuum chamber
2. p_r : partial 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_m,ss : spatial averaged metal fraction at the target surface/subsurface interface
8. n_R/n0 : relative concentration of non-reacted implanted reactive gas atoms at the target surface/subsurface interface
9. Q_p : reactive gas flow pumped away by the vacuum pump
10. Q_s : reactive gas flow consumed by compound formation on the substrate
11. Q_t : reactive gas flow consumed (> 0) or released (< 0) by the target
12. V : discharge voltage
13. I : discharge current
14. I_ion : ion current to the target
15. S : pumping speed of the vacuum pump

my_first_RSD_simulation_hyst_steady.out - Notepad

File Edit Format View Help

# Q_r[sccm](1)	p_r[Pa](2)	theta_s(3)	theta_m(4)	theta_c(5)	theta_r(6)	theta_m,ss(7)	n_R/n0(8)	Q_p
0.515801	0.001	0.190233	0.983493	0.00616335	0.0103438	0.99895	0.0105712	0.0
0.964403	0.00232667	0.35803	0.961661	0.0140218	0.0243168	0.997481	0.0248554	0.0
1.26299	0.00365333	0.471977	0.939872	0.0215181	0.0386097	0.995918	0.0394504	0.0
1.47382	0.00498	0.554403	0.91813	0.0286536	0.0532164	0.994255	0.054371	0.1
1.62889	0.00630667	0.616797	0.89641	0.0354285	0.0681618	0.992483	0.069636	0.1
1.74631	0.00763333	0.665673	0.874693	0.0418423	0.0834651	0.990593	0.0852672	0.2
1.83711	0.00896	0.704999	0.852958	0.0478941	0.099148	0.988573	0.101287	0.2
1.90835	0.0102867	0.737331	0.831184	0.0535818	0.115235	0.986412	0.117722	0.2
1.96478	0.0116133	0.76439	0.809345	0.0589029	0.131752	0.984096	0.134603	0.3
2.00968	0.01294	0.787377	0.787415	0.0638534	0.148732	0.981608	0.151963	0.3
2.04537	0.0142667	0.807158	0.765363	0.0684283	0.166209	0.97893	0.169843	0.3
2.07357	0.0155933	0.82437	0.743156	0.0726214	0.184223	0.976039	0.188287	0.4
2.09551	0.01692	0.839495	0.720754	0.0764246	0.202822	0.972909	0.207347	0.4
2.11213	0.0182467	0.852906	0.698113	0.079828	0.222059	0.969509	0.227086	0.4
2.12408	0.0195733	0.864894	0.67517	0.0828179	0.242012	0.965801	0.24758	0.5
2.13188	0.0209	0.875689	0.651879	0.0853806	0.262741	0.961738	0.268916	0.5
2.13586	0.0222267	0.88548	0.628157	0.0874961	0.284347	0.957263	0.291203	0.5
2.13624	0.0235533	0.894423	0.603914	0.0891402	0.306945	0.952302	0.314576	0.6
2.13309	0.02488	0.902647	0.579036	0.0902822	0.330682	0.946761	0.339207	0.6
2.12636	0.0262067	0.910266	0.553377	0.0908821	0.355741	0.940515	0.365317	0.7
2.11586	0.0275333	0.917377	0.526744	0.0908876	0.382368	0.933393	0.393203	0.7
2.1012	0.02886	0.924074	0.498879	0.0902272	0.410894	0.925155	0.423272	0.7

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 a 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 Windows Command Prompt and runs the `RSD2013.exe` executable with as single argument the absolute or relative 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)

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 is the simulation list window which 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 and icon is explained below.

File

Open 

To open or load an existing main input file for editing. Made changes will be saved to this opened main input file and its referenced additional 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 additional input files. Made changes to these additional input files will as such effect the original.

New 

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

Hotkey: Ctrl+N

Save 

To save the changes made in the window tabs to the main and additional 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 simulation list window, 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 additional input files. The main input file is added to the simulation list.

Exit

To exit and close the GUI window. It will not terminate any running simulation.

Simulation

Run selected 

To run the selected (blue highlighted) simulations of the simulation list in sequence.

Hotkey: Ctrl+R

Run all

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

Auto prefix

When checked, 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 they are listed. Numbering starts from 000.


When two or more items in the simulation 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

Manual 

To open the this documentation in a browser.

About

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

Tabs

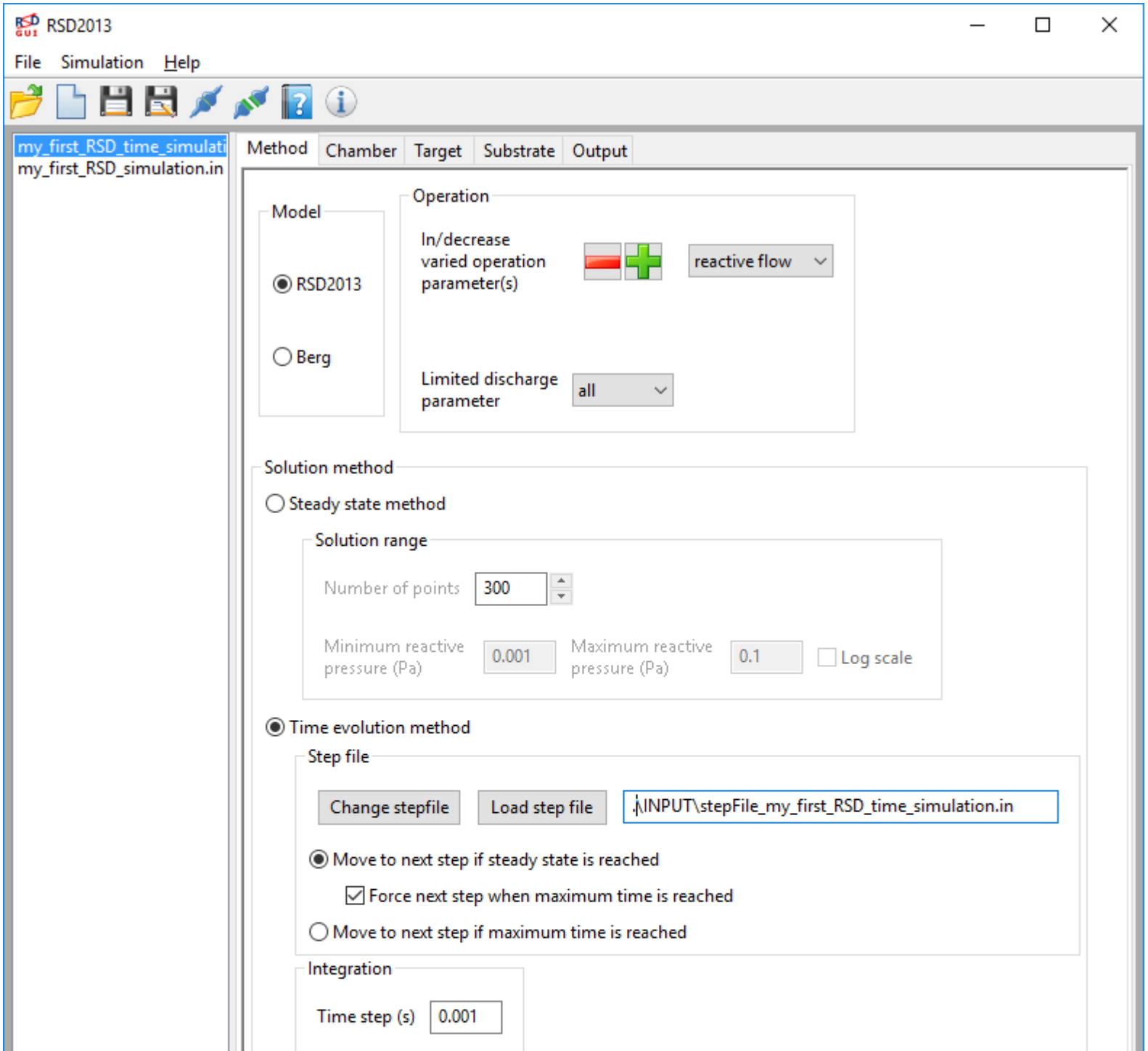
The window tabs graphically represent the information contained in the input files of a selected (blue highlighted) simulation in the simulation list. Editing the fields of these tabs changes the simulation input and options.

All simulation options are visual within the window tabs. Unused or irrelevant options or fields are grayed out and made inaccessible. They become (in)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.

Only a limited control on the input values is performed. Faulty input may crash the software at any moment and is up to the users responsibility.

Method

The window tab `Method` basically specifies which model(s) should be used, which kind of solution method is applied,how the process curve is operated and optional where to find the SiMTra simulation software.


RSD2013
File
Simulation
Help
my_first_RSD_time_simulati
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Model
RSD2013
Berg
Operation
In/decrease varied operation parameter(s)
reactive flow
Limited discharge parameter
all
Solution method
Steady state method
Solution range
Number of points
300
Minimum reactive pressure (Pa)
0.001
Maximum reactive pressure (Pa)
0.1
Log scale
Time evolution method
Step file
Change stepfile
Load step file
.\INPUT\stepFile_my_first_RSD_time_simulation.in
Move to next step if steady state is reached
Force next step when maximum time is reached
Move to next step if maximum time is reached
Integration
Time step (s)
0.001

Method window tab.

Model

- `RSD2013`

  This model is an extension of the Berg model with as most important extra feature the subsurface implantation of reactive gas ions/atoms and a 2nd order reaction mechanism in the subsurface forming the compound. A chemisorption mechanism governs the reaction on the surface. Redeposition of sputtered material back on the target can be taken into account.

- `Berg`

  This model is a monolayer surface model which only considers a chemisorption mechanism on the target (and substrate) surfaces. No redeposition can be considered.

Operation

The process curve with possible hysteresis behavior is simulated as function of a `Varied operation parameter(s)` while other operation parameters are kept fixed and specified under `Chamber`>`Operation conditions`. The plasma discharge is characterized by the operation discharge parameters `Discharge voltage`, `Discharge current` and `Discharge power` where one discharge parameter can be fixed or all.

- `Varied operation parameter(s)`
  The operation parameter(s) that will vary along the process curve/hysteresis. Multiple operation parameters can only be varied in the `Time evolution method`.
  Choices are
  - `reactive flow` (sccm)
  - `pump speed` (Ls^{-1}) **[RSD only]**
  - `voltage` (V) **[RSD only]**
  - `current` (A)**[RSD only]**
- `Limited discharge parameter`
  The discharge parameter(s) that is (are) kept fixed along the process curve/hysteresis, specified in `Chamber`>`Operation conditions`.
  - `voltage`, `current` or `power` **[RSD only]**
    The discharge parameter that has a fixed value. The other discharge parameters are determined by the `IV-characteristics`.
  - `all` :
    All discharge parameters have a fixed value.

- `N/A` **[RSD only]**
  All discharge parameters are determined by the `IV-characteristics`.
  Only if `all` is chosen, their is no need for specifying `Chamber`>`IV-characteristics`.
  If the `Berg` model is chosen, only the option `Varied operation parameter`>`reactive flow` with `Limited discharge parameter`>`all` is currently possible.

Solution method

As solution method, two options are available the `Steady state method` and the `Time evolution method`.

- `Steady state method`
  The chosen `Model` will be solved as a steady state model (with time derivatives set to zero) to simulate the process curve/hysteresis. It simulates the entire process curve/hysteresis including the potential unstable regions. The independent variable p_r (or V) is first stepwise increased (or decreased) over the `Solution range` and subsequently decreased (or increased).
  - `Solution range`
    - `Number of points` :
      The total number of simulated points along the process curve/hysteresis. Each value of the independent variable is simulated twice. Once for the increasing and once for the decreasing direction.
    - `Minimum reactive pressure (Pa)` or `Minimum voltage (V)` :
      Lower bound for the independent variable based on the `Varied operation parameter` choice.
    - `Maximum reactive pressure (Pa)` or `Maximum voltage (V)` :
      Upper bound for the independent variable based on the `Varied operation parameter` choice.
    - `Log scale` :
      Distributes the simulation points logarithmic between lower and upper bound (default: linearly).

      If a range of discharge voltage is requested, the steady state solver will translate this to a conform reactive pressure range to use as independent variable and solve the model. In this way, the specified discharge voltage range will not coincidence with the output range.

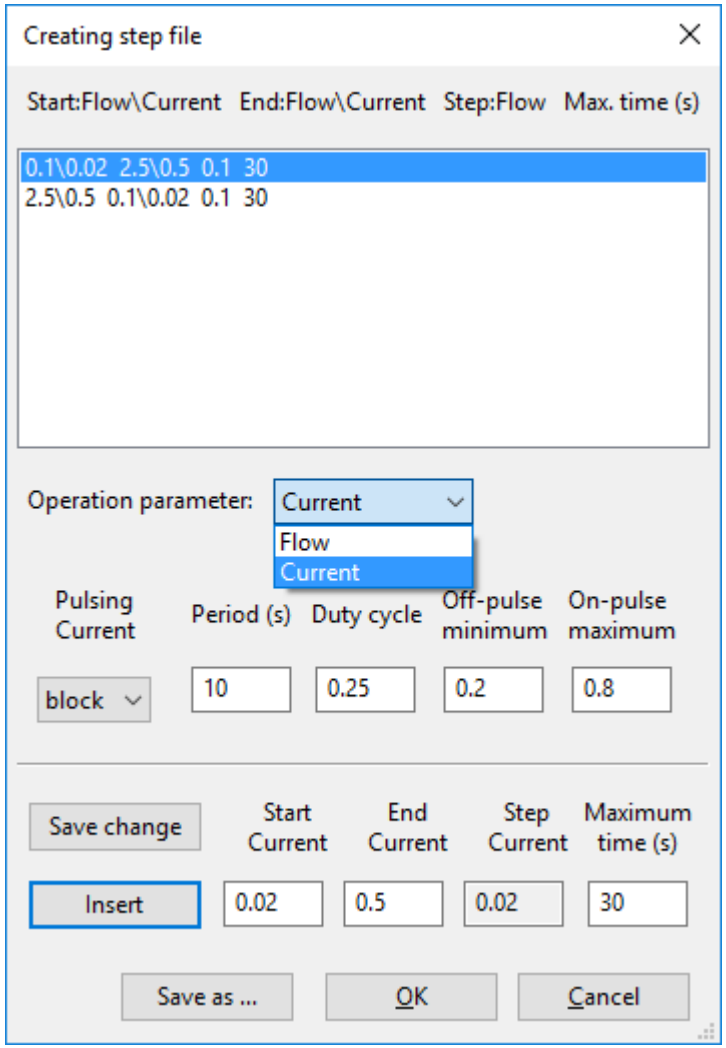
- `Time evolution method`
  The chosen `Model` will be solved as a time dependent model. The `Varied operation parameter(s)` is (are) stepwise in- or decreased with an optional periodic pulsing accordingly the specifications in the `Step file`.
  - `Step file`
    The created step file is an additional input file and defines the predefined evolution of the `Varied operation parameter(s)`.
    - `New step file` or `Change step file` :
      Opens the window `Creating step file` where a new or existing step file can be modified.

- `Loading step file` :
  Allows to choose the path of an existing step file which will be represented in the text field. Direct editing of this text field is also possible.
- `Move to next step if steady state is reached` :
  Initiates the next `Varied operation parameter(s)` value only when the process reaches a steady state condition, even a periodic steady state in case of `Pulsing` of at least one of the `Varied operation parameter(s)`. If `Force to next flow if maximum time is reached` is enabled, it initiates the next `Varied operation parameter(s)` when steady state is reached OR when the maximum time for this set value of the `Varied operation parameter(s)` is reached.
- `Move to next step if maximum time is reached` :
  Initiates the next `Varied operation parameter(s)` value only when the maximum time for the current `Varied operation parameter(s)` value is reached.

o `Integration`

- `Time step` (s) :
  It defines the integration step Δt of the explicit 4th order Runge-Kutta integrator which numerically solves the ordinary differential equations of the variables θ_m, θ_c, θ_r, θ_s and p_{ir}, and optional I and V.

Creating step file

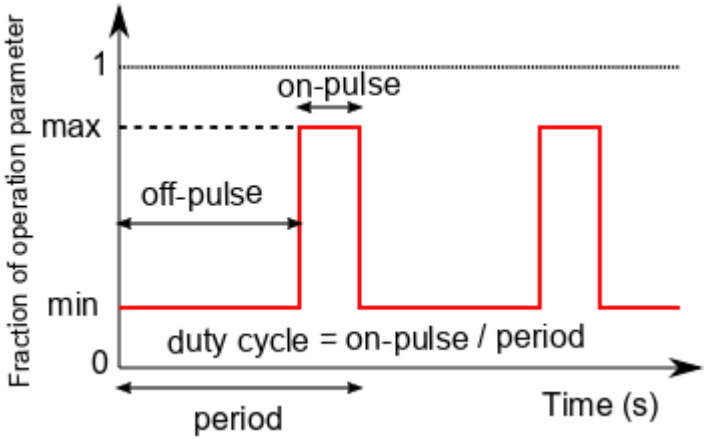


Window Creating step file

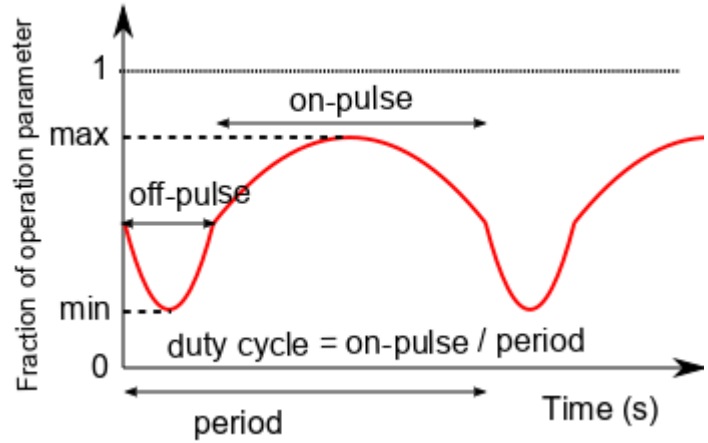
A step file consist of a list numerical text lines which define a stepwise in/decrease of each of the specified `Varied operation parameter(s)`. Each line consist out of four entries:

- `Start` :
  The start value of the listed `Varied operation parameter(s)` as a '\' separated string.

- `End` :
  The end value of the listed `Varied operation parameter(s)` as a '\' separated string.
- `Step` :
  The value with which the `Start` value of the first listed `Varied operation parameter(s)` is stepwise in/decreased until it reaches the `End` value. The other `Varied operation parameter(s)` their `Step` is defined by the stepping of this first listed `Varied operation parameter(s)`.
- `Maximum time (s)` :
  The maximum time each stepped value of the `Varied operation parameter(s)` is set during the 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 `Delete`, the line is removed.
  By double clicking, the line is selected and loaded in the editing fields. The `Varied operation parameter(s)` that needs to be changed, is selectable next to `Operation parameter:`. Only the `Step` of the first listed operation parameter can be edited as the other step are defined by this `Step`. After making changes to the line, you can press the `Save change` button to save the changes to the original line.
- `Pulsing`
  Optional one or more of the `Varied operation parameter(s)` can have a pulse character as
  - `NA`:
    No pulsing of the selected `Operation parameter`.
  - `block`:
    The selected `Operation parameter` is block pulsed, shaped by the parameters below and given in the figure.
  - `sinus`:
    The selected `Operation parameter` has a sinusoidal form, shaped by the parameters below and given in the figure.
    - `Period (s)` :
      The total time of a single period
    - `Duty cycle` :
      Fraction (0 to 1) of the period where the `Varied operation parameter(s)` reaches its scaled `Maximum` value.
    - `Off-pulse minimum` :
      Relative scaling of the `Varied operation parameter(s)` during the off-time or minimum of the pulse which precedes the on-time or maximum of the pulse.
    - `On-pulse maximum` :
      Relative scaling of the `Varied operation parameter(s)` during the on-time or maximum of the pulse which comes after the off-time or minimum of the pulse.



Definition of block pulsing of operation parameters.



Definition of sinusoidal pulsing of operation parameters.

Pressing the `Ok` button save the change to loaded step file or pops up a window to specify a saving location if no step file is loaded yet. A default name is suggested. It is a concatenation of the string `stepFile` with the name of the main input file.
`Save as ...` allows to save the stepping as a new step file and replace the original loaded step file.

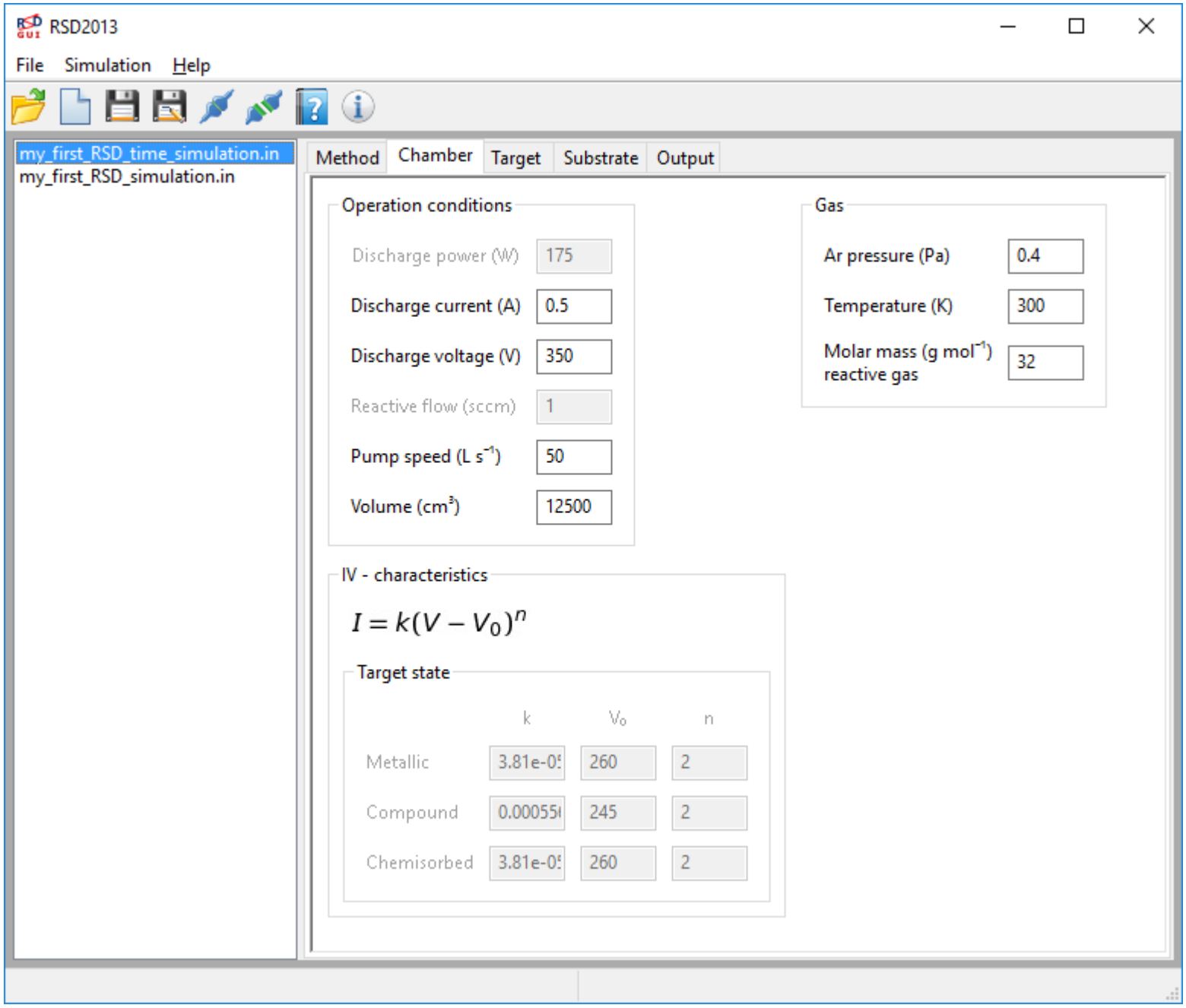
SiMTra

If SiMTra simulated deposition profiles should be included, the SiMTra home directory has to be specified. This version of RSD is compatible with SiMTra v2.2 which accompanies the RSD2013 software.

- `Use SiMTra deposition simulations`
  If checked, SiMTra simulated deposition profiles can be simulated and/or included. The SiMTra home directory containing the executables `simtra_gui.exe` and `simtra_cmd.exe` should be specified with its absolute or relative path in the text field.
  - `Synchronise RSD with SiMTra input`
    If checked, the parameters defined by the SiMTra input file will be transferred to the RSD software and the relevant parameter fields will be made non-editable. The following simulation parameters will be synchronized with SiMTra:
    - `Volume` (cm^3)
      It will import the volume of the chamber object defined in SiMTra as it is completely empty.
    - `Ar pressure` (Pa)
      It will import the defined gas pressure.
    - `Temperature` (K)
      It will import the defined gas temperature.
    - Target `Area` (cm^2)
      It will import the area of the surface object that is assigned to sputter.
    - Substrate `Area` (cm^2)
      It will import the total sum of all defined surface objects where deposition is recorded.
  - `Run SiMTra within RSD simulation`
    If checked, the SiMTra simulation as specified by the SiMTra input file in the window tab `Target`>`Metal particle M`>`Simtra` for the deposition profile of the sputtered metal will (re)started before the effective RSD simulation is performed.
    If not checked, the SiMTra simulation should have been executed before as the output is expected to reside on the location given by the SiMTra input file.
  - `Enable movement`
    A periodic movement should be specified in the SiMTra simulation.
    - `full period`
      The end of a period is followed by its start.
    - `half period`
      At the end of a period the movement reverse in direction towards its start where it reverse again.

Chamber

The window tab `Chamber` specifies the parameters connected to the gases in the chamber, the fixed operation conditions and the IV-characteristics for the different target states.


RSD2013
File
Simulation
Help
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Operation conditions
Discharge power (W)
175
Discharge current (A)
0.5
Discharge voltage (V)
350
Reactive flow (sccm)
1
Pump speed (L s-1)
50
Volume (cm3)
12500
Gas
Ar pressure (Pa)
0.4
Temperature (K)
300
Molar mass (g mol-1) reactive gas
32
IV - characteristics
$I = k(V - V_0)^n$
Target state
k
V0
n
Metallic
3.81e-05
260
2
Compound
0.00055
245
2
Chemisorbed
3.81e-05
260
2

Chamber tab window.

Operation conditions

The discharge operation parameters and chamber conditions.

- `Discharge power` (W) **[RSD only]**
  A fixed electrical power *P* for the discharge. To be specified if `Limited discharge parameter` is `power`.
- `Discharge current` (A)
  A fixed electrical current *I* for the discharge. To be specified if `Limited discharge parameter` is `current` or `all`.
- `Discharge voltage` (V)
  A fixed electrical voltage *V* for the discharge. To be specified if `Limited discharge parameter` is `voltage` or `all`.
- `Reactive flow` (sccm) **[RSD only]**
  A fixed reactive flow Q_r introduced into the vacuum chamber. To be specified if `Varied operation parameter(s)` is `pump`, `current` or `voltage`.
- `Pump speed` (L s^{-1})
  A fixed volumetric pumping speed *S* of the reactive gas out of the vacuum chamber. To be specified if `Varied operation parameter(s)` is `reactive flow`, `current` or `voltage`.

  
  The system pumping speed can be determined as the slope of the steady state Q_r-p_r relation when the discharge is off. For correctness, the fixed Ar gas pressure should be established, as the pumping speed may depend on the gas mixture.
- `Volume` (cm^3)
  A fixed volume *V* of the vacuum chamber which occupies the gases. Only relevant for the `Time evolution method`.

  
  The volume of the vacuum chamber can be estimated based on the time evolution of the gas pressure p_r when the gas flow Q_r is changed. Knowledge of the pumping speed and gas temperature is then required.

Gas

Parameters specifying the used reactive gas, the global gas temperature and Ar pressure.

- `Ar pressure` (Pa) **[RSD only]**
  The fixed and constant pressure p_{Ar} of the inert argon gas in the vacuum chamber.
- `Temperature` (K)
  The fixed and constant temperature *T* of the reactive and inert Ar gas.

- `Molar mass reactive gas` (g mol^{-1})
  Specifies the used diatomic molecular reactive gas by its molar mass.

IV-characteristics [RSD only]

If the `Limited discharge parameter` is not set to `all`, three current-voltage characteristics (IV-characteristics) should be specified for the target in a complete `Metallic`, `Compound` or `Chemisorbed` state at the specified `Ar pressure (Pa)`. These IV-characteristic are highly system dependent (magnetic field configuration, gas pressure, inert gas type). Each IV-characteristic has the form:

$$I = k(V - V_0)^n$$

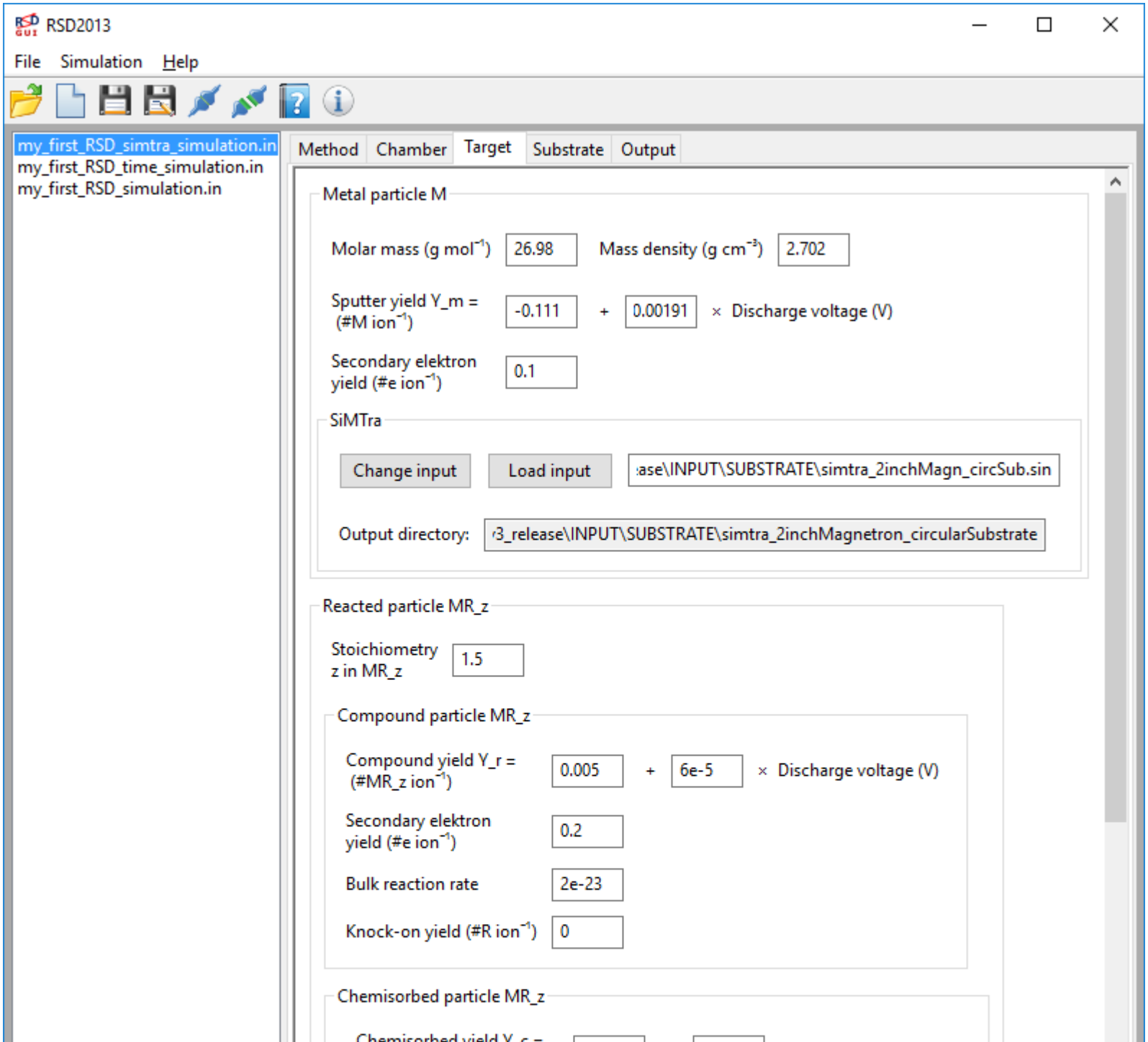
with the parameters k, V_0 and n depending on the `Target state`.

IV-characteristics for magnetrons are often well fitted by the Westwood relation www (n=2).

While IV-characteristics for a `Metallic` and a `Compound` target state can often been measured, this is not the case for a `Chemisorbed` target state. This chemisorbed IV-characteristic may be a fitting element or equally set like the metallic or compound IV-characteristic.

Target

The window tab `Target` specifies the properties and interaction mechanisms of the particles on the target surface and subsurface. There are the sputtered particles (M and MR_z), the deposited particles (M and R) and the implanted particles (R_2^+). It also specifies the geometry of the sputtered target and optional if redeposition of sputtered material back on the target should be considered.


RSD2013
File
Simulation
Help
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Metal particle M
Molar mass (g mol-1)
26.98
Mass density (g cm-3)
2.702
Sputter yield Y_m = (#M ion-1)
-0.111
+
0.00191
× Discharge voltage (V)
Secondary elektron yield (#e ion-1)
0.1
SiMTra
Change input
Load input
ase\INPUT\SUBSTRATE\simtra_2inchMagn_circSub.sin
Output directory:
3_release\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate
Reacted particle MR_z
Stoichiometry z in MR_z
1.5
Compound particle MR_z
Compound yield Y_r = (#MR_z ion-1)
0.005
+
6e-5
× Discharge voltage (V)
Secondary elektron yield (#e ion-1)
0.2
Bulk reaction rate
2e-23
Knock-on yield (#R ion-1)
0
Chemisorbed particle MR_z

Target tab window tab (part 1).

Metal particle M

- `Molar mass` (g mol^{-1})
  Specifies the sputtered metal element M by its molar mass.
- `Mass density` (g cm^{-3})
  Specifies the sputtered metal element M by its mass density.
  A metal particle density n_0 is calculated from the `Mass density` and the `Molar mass`. This density n_0 is the metal density in the target, independent if the metal is in a bounded or unbounded state with reactive atoms.
- `Sputter yield Y_m` (#M ion^{-1})
  The sputter yield of metal particles M per incoming ion if the metal is not bounded with reacitve atoms (metallic state). This can optional be specified as a linear function of the discharge voltage. No distinction is made between inert or reactive incoming ions.
  Metal sputter yields can be measured by a weighting or volume method but can also be simulated with Monte Carlo codes like SRIM www.
- `Secondary electron yield` (#e ion^{-1})
  The ion-induced secondary electron emission yield for non-reacted metal. If different from zero, the discharge current is considered to have an ion and an electron contribution. Otherwise discharge and ion current are assumed equal.
  Secondary electron yields of metals can be retrieved from Depla et al. www.
- `SiMTra`
  If SiMTra deposition profiles of the sputtered metal are considered, the SiMTra input file should be specified or a new SiMTra simulation has to be set up.
  A loaded SiMTra input file will represent the target surface in `Target`> `Geometry`> `Redeposition profile`> `SiMTra configuration`> `Object`/`Surface` and the substrate surfaces in `Substrate`> `Geometry`> `Deposition profile`> `SiMTra configuration`> `Object`/`Surface`.
  To load or set up such a SiMTra input file, one can use
  - `New input` or `Change input`
    If the adjacent text field does not contain an absolute or relative path to a valid SiMTra input file, the `New input` will start up the SiMTra GUI to compose a new SiMTra simulation configuration. After saving this SiMTra configuration and closing the SiMTra GUI, the last saved SiMTra input file will be shown in the adjacent text field.
    If the adjacent text field does contain an absolute or relative path to a valid SiMTra input file, the `Change input` will start up the SiMTra GUI to edit the existing SiMTra simulation configuration.
    When a
  - `Load input`
    Browse for an existing SiMTra input file which will be shown in the adjacent text field.

- `Output directory`
  Non editable text field which shows the output directory for the SiMTra simulation. This output directory is only editable in the SiMTra GUI or the SiMTra input file.
   If the text field of `Output directory` is empty, their is no valid SiMTra input file specified.

Reacted particle particle MR_z

Two types of reacted metal particles are considered. Compound particles are formed in the subsurface by reaction of implanted reactive gas ions and the metal atoms which come to the surface by sputter erosion. Chemisorbed particles are formed on the surface due to the chemisorption of the molecular reactive gas on non-reacted metal atoms. Reaction and particle specific parameters should be specified here.

- `Stoichiometry z in MR_z`
  The stoichiometric factor *z* as the number of reactive gas atoms R bounded on a metal atom M. This stoichiometric factor is the same for all reacted metal particles as well on the target as on the substrate.
   In principle the model can only handle compounds with a single oxidation state like Al_2O_3, Y_2O_3 and MgO.
- `Compound particle MR_z` **[RSD only]**
  - `Sputter yield Y_r` (#M ion^{-1})
    The sputter yield of compound particles MR_z per incoming ion if the metal is bounded with reactive atoms (compound state). This can optional be specified as a linear function of the discharge voltage. No distinction is made between an incoming inert or reactive ions.
     By definition the compound sputters congruently (=maintaining the existing stoichiometry) but are sputtered as atoms.
     Effective compound sputter yields can be measured by a weighting or volume method. Simulation by Monte Carlo codes like SRIM www require suitable surface binding energies of the components and reproduce ‘pure’ sputter yield without the effect of dilution by the implanted gas concentration. Gas consumption measurements as proposed by Schelfhout et al. www give good estimates for these effective sputter yield.
  - `Secondary electron yield` (#e ion^{-1})
    The ion-induced secondary electron emission yield for compound. If different from zero, the discharge current is considered to have an ion and an electron contribution. Otherwise discharge and ion current are assumed equal.
     Secondary electron yields of compounds can be retrieved from Depla et al. www.
  - `Bulk reaction rate` ($cm^3s^{-1}\#R^{-1}$) The 2nd order reaction rate coefficient for the formation of compound particles MR^z in the subsurface from implanted reactive gas ions and non-reacted metal atoms.
     The reaction rate is in close relationship with the compound sputter yield, and both parameters dominate the position of the second critical point. It may be considered as a fit parameter. More info www, www.

- `Knock-on yield` (#R ion^{-1}) The knock-on yield of reactive gas atoms in the compound state. It is the yield of reactive atoms that are knocked of from a compound particle at the surface into the target subsurface by an incoming inert or reactive ion.

  Note that the used `Bulk reaction rate` values in RSD literature are conform with a zero `Knock-on yield` for the compound particle. If non-zero values are used, the `Bulk reaction rate` should probably be increased.

- `Chemisorbed particle MR_z`
- `Sputter yield Y_c` (#M ion^{-1})

  The sputter yield of chemisorbed particles MR_z per incoming ion if the metal is chemisorbed by reactive atoms (chemisorbed state). This can optional be specified as a linear function of the discharge voltage. No distinction is made between an incoming inert or reactive ions.

  By definition the chemisorbed particles sputter congruently (=maintaining the existing stoichiometry) but are sputtered as atoms.

  No good estimates of sputter yields for chemisorbed particles are known, but are expected to lay between the metal and the compound sputter yield.
- `Secondary electron yield` (#e ion^{-1})

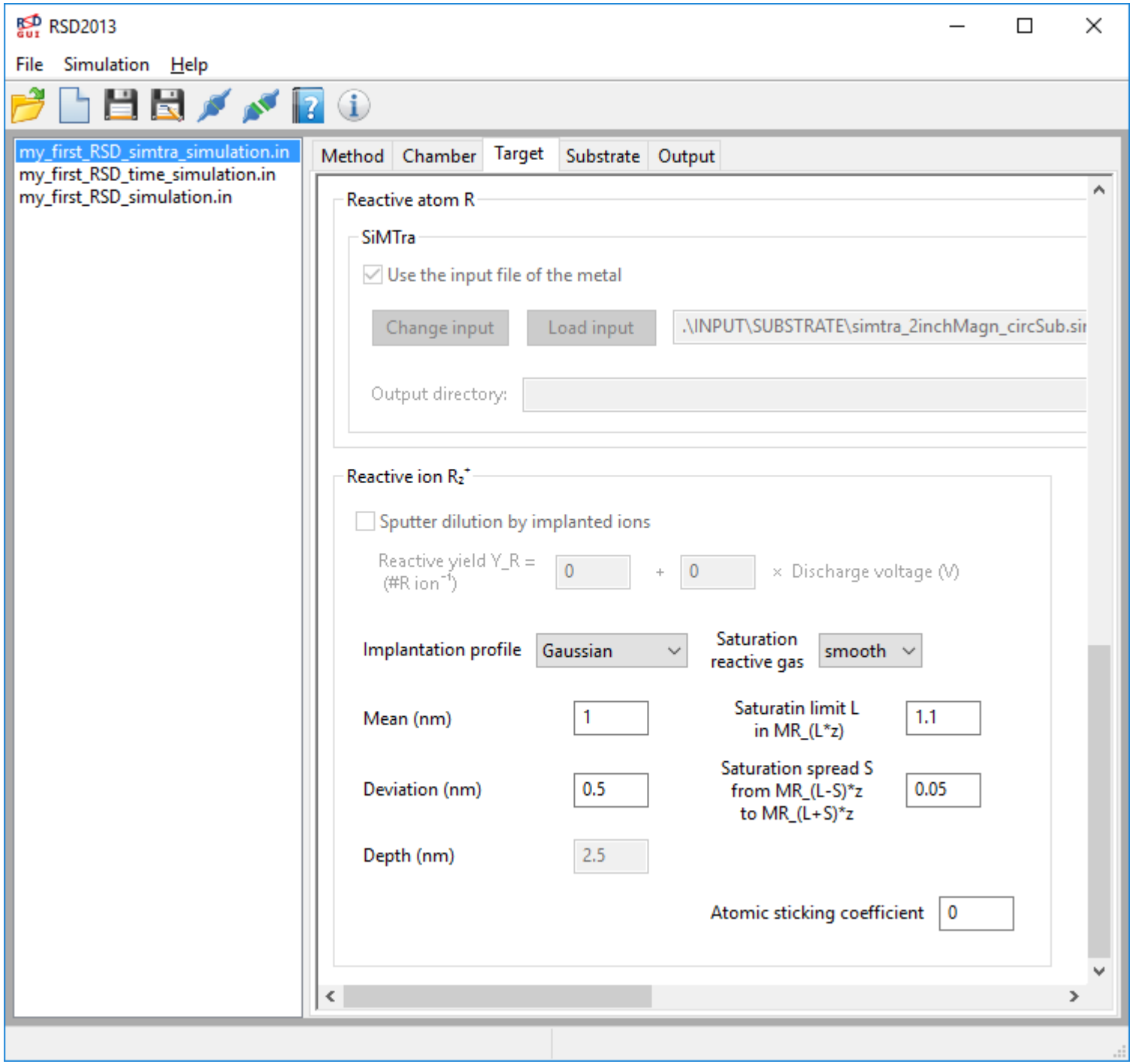
  The ion-induced secondary electron emission yield for the chemisorbed state. If different from zero, the discharge current is considered to have an ion and an electron contribution. Otherwise discharge and ion current are assumed equal.

  No good estimates for the secondary electron yields of chemisorbed states are known, but should be typical lower than the metal state.
- `Effective sticking coefficient`

  The effective sticking coefficient of non-sputtered reactive gas. It is the average probability for a gaseous reactive particle (atom or molecule) to chemisorb on a metallic surface to form a chemisorbed particle.

  No good estimates for the effective sticking coefficient on the target are known. Typically the same sticking coefficient as for the substrate may be used.
- `Knock-on yield` (#R ion^{-1}) The knock-on yield of reactive gas atoms in the chemisorbed state. It is the yield of reactive atoms that are knocked of from a chemisorbed particle at the surface into the target subsurface by an incoming inert or reactive ion.

  Knock-on yield may be estimated with Monte Carlo codes like SRIM www by defining a monolayer of oxygen on the metal and calculating the knock-on probability.


RSD2013
File
Simulation
Help
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Reactive atom R
SiMTra
Use the input file of the metal
Change input
Load input
.\INPUT\SUBSTRATE\simtra_2inchMagn_circSub.si
Output directory:
Reactive ion R2+
Sputter dilution by implanted ions
Reactive yield Y_R = (#R ion-1)
0
+
0
× Discharge voltage (V)
Implantation profile
Gaussian
Saturation reactive gas
smooth
Mean (nm)
1
Saturatin limit L in MR_(L*z)
1.1
Deviation (nm)
0.5
Saturation spread S from MR_(L-S)*z to MR_(L+S)*z
0.05
Depth (nm)
2.5
Atomic sticking coefficient
0

Target window tab (part 2).

Reactive atom R

Not implemented yet.

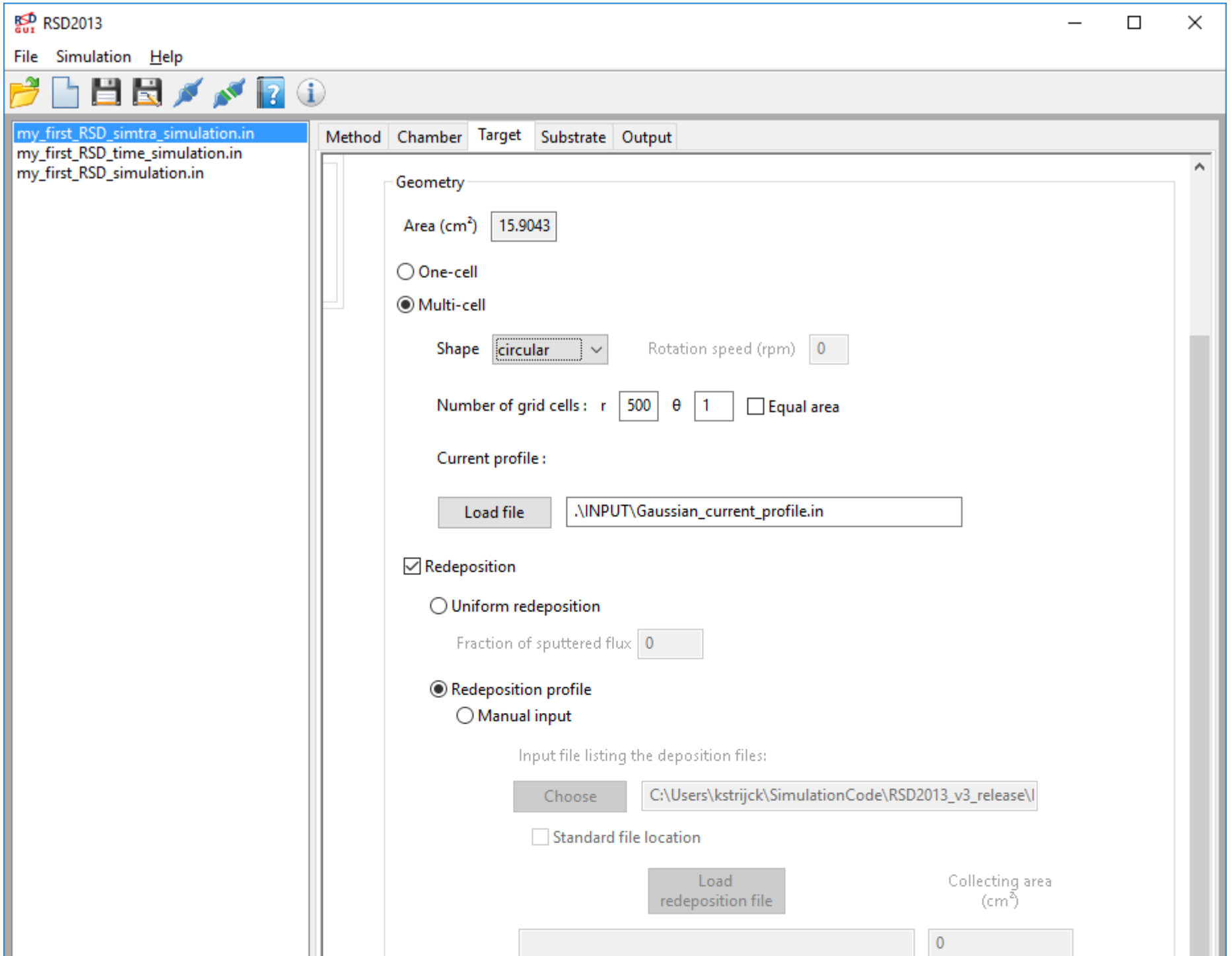
Reactive ion R_2^+ [RSD only]

- `Sputter dilution by implanted ions`
  If checked, the concentration of implanted reactive gas ions at the target surface will decrease the sputter yield of all (reacted) metal and all reactive atoms proportional with their relative concentration.
  `Sputter dilution by implanted ions` is only optional if the `Time evolution method` is chosen.
  Bear in mind that now 'pure' sputter yield for all particles (metal, compound and chemisorbed) are required as Monte Carlo codes like SRIM www ideally produce if this effect is not accounted for.
  - `Reactive yield Y_r` (#R ion^{-1})
    The sputter yield of non-reacted implanted reactive gas ions R per incoming ion. This can optional be specified as a linear function of the discharge voltage. No distinction is made between an incoming inert or reactive ions.
    Sputter yield of unbounded reactive gas in a metal can be estimated by Monte Carlo codes like SRIM www by defining a target with an equal metal as reactive gas density and setting the reactive gas surface binding energy zero.
- `Implantation profile`
  Reactive ions get direct or knock-on implanted in the subsurface of the target according a specific spatial distribution. For both mechanisms, the same implantation profile is assumed.
  Implantation profiles and depth ranges can be estimated with Monte Carlo codes like SRIM www.
  - `Gaussian`
    A Gaussian or normal implantation distribution that is cut off at a depth of μ + 3σ.
    - `Mean (nm)` The mean μ of the Gaussian implantation profile.
    - `Deviation (nm)` The deviation σ of the Gaussian implantation profile.
  - `uniform`
    A uniform implantation distribution covering a specific `Depth (nm)`.
  - `uniform (fast)` A uniform implantation distribution covering a specific `Depth (nm)`, but less computational intensive as the analytical solution for the subsurface is used.
    `uniform (fast)` is only applicable if the `Steady state method` is chosen.

- `Depth (nm)`
  The implantation range if a `uniform` or `uniform (fast)` implantation profile is chosen.
- `Saturation reactive gas`
  A limitation on the reactive gas implantation in the subsurface of the target can be enforced if the subsurface reactive gas concentration exceeds a certain maximum. This maximum concentration is the sum of non-reacted and reacted reactive gas atoms in the subsurface. The possible overdose of implanted reactive gas atoms is then assumed to directly diffuse out of the target. The implantation limitation is established by a saturation function which takes the form of an error function. This saturation function scales the implantation dose based on the local reactive gas concentration.

   Estimates for the saturation concentrations of the reactive gas are hard. Feel free to use it as your favorite fit parameter.
  - `non`
    No saturation function is applied. All implanted reactive gas reside in the target subsurface.
  - `abrupt`
    A sharp limitation on the reactive gas implantation applies as the saturation/error function is centered around the limiting concentration *L*z* reactive atoms per metal atom with a ‘spread’ of zero.
- `Saturation limit L in MR_(L*z)`
  The limitation *L* as *L*z* of reactive gas atoms per metal atom.
  - `smooth`
    A smooth limitation on the reactive gas implantation applies as the saturation/error function is centered around the limiting concentration *L*z* reactive atoms per metal atom with a ‘spread’ *S*z*.
- `Saturation spread S from MR_(L-S)*z to MR_(L+S)*z`
  The smoothness *S* as *S*z* of reactive gas atoms per metal atom.
- `Atomic sticking coefficient`
  If non-zero, out-diffusing and/or surface reaching implanted reactive gas atoms may chemisorb on non-reacted metal atoms at the target surface with the specified probability.

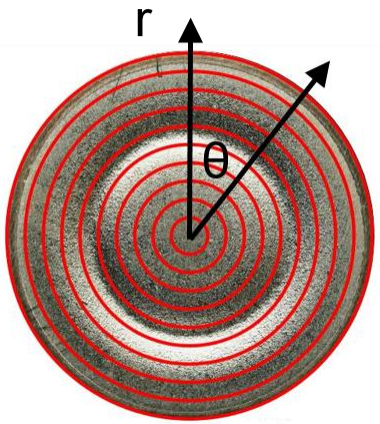
   Gas atoms are highly reactive, while gas molecules are less reactive. This sticking coefficient represent both species and should be estimated depending on the assumed ratio of both types.


RSD2013
File
Simulation
Help
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Geometry
Area (cm²)
15.9043
One-cell
Multi-cell
Shape
circular
Rotation speed (rpm)
0
Number of grid cells : r
500
θ
1
Equal area
Current profile :
Load file
.\INPUT\Gaussian_current_profile.in
Redeposition
Uniform redeposition
Fraction of sputtered flux
0
Redeposition profile
Manual input
Input file listing the deposition files:
Choose
C:\Users\kstrijck\SimulationCode\RSD2013_v3_release\I
Standard file location
Load redeposition file
Collecting area (cm²)
0

Target window tab (part 3).

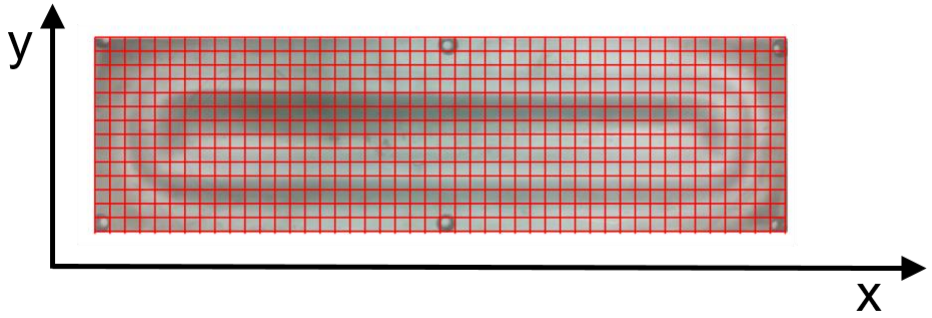
Geometry

- `Area` (cm²)
  The surface area of the sputtered target. For a `One-cell` target, this corresponds with the effective eroded surface area (racetrack). For a `Multi-cell` target, this corresponds with the surface area where for a `Current profile` is specified below.
- `One-cell`
  The `One-cell` description considers the target spatial 1-dimensional. It is spatial uniform in the lateral (x/r-y/θ) directions but spatial resolved in the longitudinal (z) direction. The ion current density on the target surface is uniform as well as the state of the target in the lateral directions.
- `Multi-cell`
  The `Multi-cell` description considers the target spatial 3-dimensional. It is spatial resolved in both the lateral (x/r-y/θ) directions as in the longitudinal (z) direction. Specification of a `Current profile` is obligatory.
  - `Shape`
    Two geometrical shapes of the target are selectable, each with their own lateral spatial partitioning in target cells.
    - `circular`
      A planar circular target surface with a radius conform the specified `Area`.



Spatial partitioning circular target.

    - `rectangular\rotatable`
      A planar rectangular\cylindrical target surface partitioned in `x` cells along its width\circumference) and in `y` cells along its length. All target cells are equal in surface area.



Spatial partitioning rectangular target.

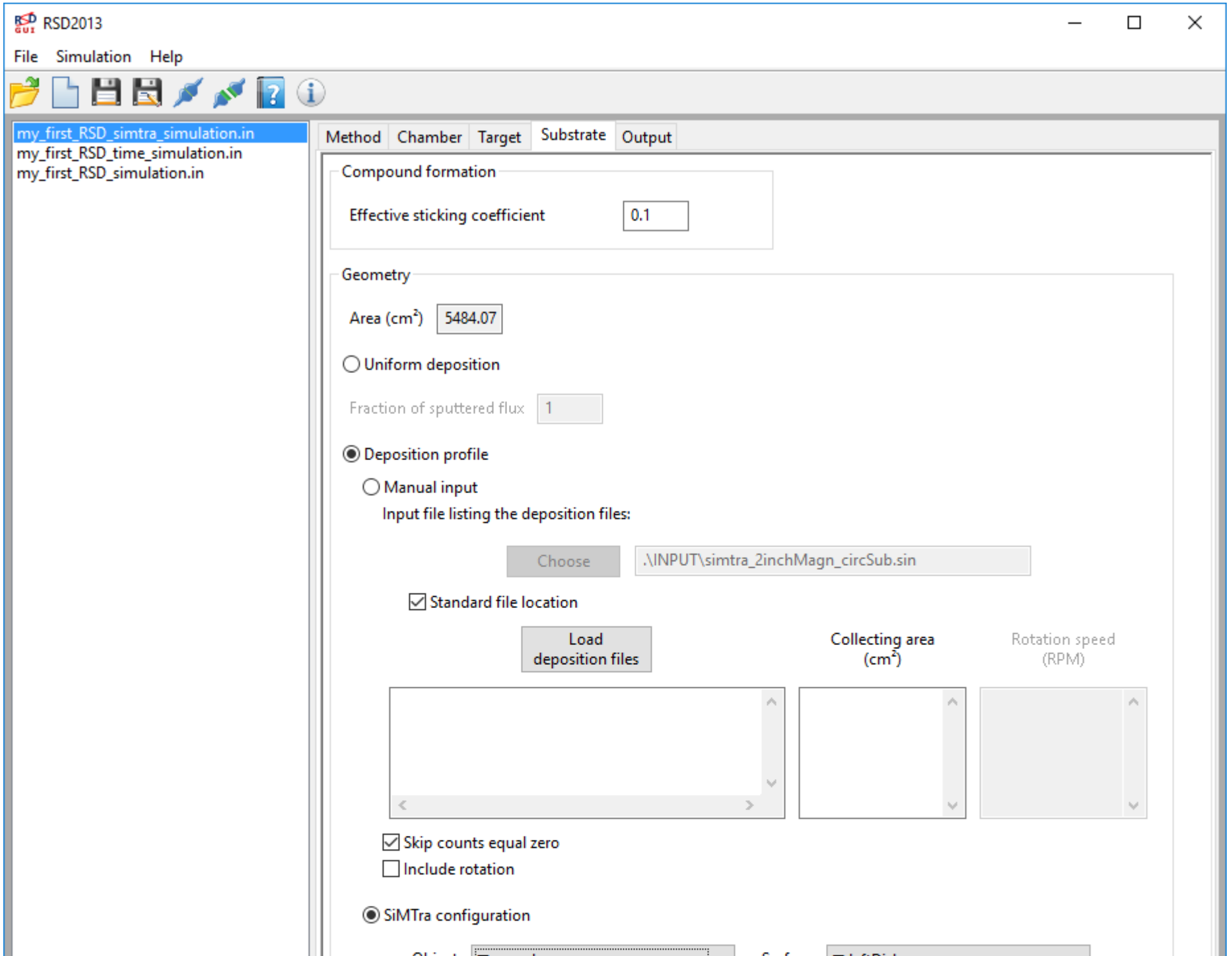
- `Rotation speed (rpm)`
  If non-zero, the `rotatable` target is assumed to be a rotating cylindrical target surface with a rotation speed in rounds per minute in the `x` dimension. This option is only applicable for a `rotatable` target.
- `Number of grid cells`
  - `r` or `x`
    For a `circular` target, the number of target cells in the radial `r` dimension.
    For a `rectangular` target, the number of target cells in the `x` dimension.
  - `θ` or `y`
    For a `circular` target, the number of target cells in the azimuthal `θ` dimension.
    As the `Current profile` for a `circular` target has to be axial symmetric, partitioning in the azimuthal dimension (θ > 1) is only useful if an asymmetric `Redeposition profile` is included.
    For a `rectangular` target, the number of target cells in the `y` dimension.
  - `Equal area`
    If checked, the `circular` target is partitioned in the radial dimension such that the target cells have all an equal surface area. Only applies for a `circular` target as the `rectangular` target is always equally partitioned.
- `Current profile`
  The relative distribution of the ion current across the target surface has to be specified by an additional input file, the current profile file, which has to be conform with the chosen `Shape` of the target. Only applies for a `Multi-cell` description of the target.
  - `Load file`
    Browse for an appropriate current profile file or directly enter its path in the adjacent text field.
- `Redeposition` **[RSD only]**
  If checked, redeposition of sputtered material back on the target shall be included.

- `Uniform redeposition`
  A spatial uniform redeposition on the target is considered.
  - `Fraction of sputtered flux`
    The fraction (between 0 and 1) of the total sputtered flux that is redeposited on the target. The same fraction is used for both the sputtered metal as the sputtered reactive atoms. Editing this fraction changes in a conform way the total fraction of the sputtered flux deposited on all substrates, presented in `Substrate`> `Geometry`> `Uniform deposition`> `Fraction of sputtered flux` or `Substrate`> `Geometry`> `Deposition profile`> `Only profile with fraction`.
- `Redeposition profile`
  A spatial resolved redeposition profile is considered, typically based on SiMTra simulations.
  - `Manual input`
    Old style manner of including the redeposition distribution on the target based on a SiMTra deposition profile file. This way of including redeposition does not need the SiMTra input file, only the deposition profile file and the spatial area it covers.
  - `Input file listing the deposition files:`
    An additional input file, the redeposition listing file, lists the single SiMTra deposition profile file that contains the redeposition distribution over the target besides the corresponding surface area. This file can be saved on the `Standard file location` or can freely be chosen by unchecking the box and editing the adjacent text field or using the `Choose` button. An already existing redeposition listing file can also be loaded in the same way.
  - `Load redeposition file`
    The location of the SiMTra deposition profile file containing the redeposition distribution can be looked up or the file location can directly be given in the text field.
  - `Collecting area`
    Each SiMTra deposition profile file defines a rectangular grid overlaying the considered surface. The area of this grid has to be provided and not the effective area of the considered surface.
  - `SiMTra configuration`
    This is the preferred way of including a redeposition distribution on the target. It is based on a SiMTra input file which should be specified in the text field under `Target`> `Metal particle M`> `SiMTra`.
    For the target, a single `Object` and `Surface` are listed. Non-editable properties of this `Object` and `Surface` are shown which can only be modified in the SiMTra GUI or the SiMTra input file.
  - `Object`
    The name of the object as defined in the SiMTra input file where the target surface is part of. The non-editable properties `Position` and `Orientation` of this object are listed.
    The symbol in front of the object name indicates if deposition profiles where saved during the SiMTra simulation and are as such included or not.
    ■ : all contained surfaces of this object have deposition profiles
    □ : all contained surfaces of this object have NO deposition profiles
    ◪ : some of the contained surfaces of this object have deposition profiles

- `Surface`
  The name of the target surface as defined in the SiMTra input file. The symbol in front of the surface name indicates if the deposition profile was saved during the SiMTra simulation and is as such included or not.
  ■ : surface has deposition profile
  □ : surface has NO deposition profile
  The non-editable properties `Type`, `Position` and `Orientation` within the local coordinate system, `Area` and `Grid resolution` are listed. Target rotation can only be specified under `Target`> `Geometry`> `Multi-cell`> `Rotation speed` if the `Shape` is a `rotatable` target.
- `Only fraction (uniform profile)`
  If checked, only the redeposition fraction as simulated by SiMTra is used and a uniform redeposition is considered.
- `Only profile with fraction`
  If checked, only the relative redepositoin profile as simulated by SiMTra are used and scaled by the given redeposition fraction. Editing this fraction changes in a conform way the total deposition fraction on all the substrates, presented in `Substrate`> `Geometry`> `Uniform deposition`> `Fraction of sputtered flux` or `Substrate`> `Geometry`> `Deposition profile`> `Only profile with fraction`.

Substrate

The window tab `Substrate` specifies the properties connected with the substrate surface and the interaction mechanisms of the reactive molecular gas with the deposited material. It specifies the deposition profile and fraction on the substrates.


RSD2013
File
Simulation
Help
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Compound formation
Effective sticking coefficient
0.1
Geometry
Area (cm²)
5484.07
Uniform deposition
Fraction of sputtered flux
1
Deposition profile
Manual input
Input file listing the deposition files:
Choose
.\INPUT\simtra_2inchMagn_circSub.sin
Standard file location
Load deposition files
Collecting area (cm²)
Rotation speed (RPM)
Skip counts equal zero
Include rotation
SiMTra configuration

Substrate window tab.

Compound formation

- `Effective sticking coefficient`
  The effective sticking coefficient of non-sputtered reactive gas . It is the average probability for a gaseous reactive particle (atom or molecule) to chemisorb on a metallic surface to form a chemisorbed particle.

  
  Effective sticking (or incorporation) coefficient can be estimated based on the electronegativity difference between the metal and the reactive gas atom in combination by the rough relation found by Leroy et al. www

Geometry

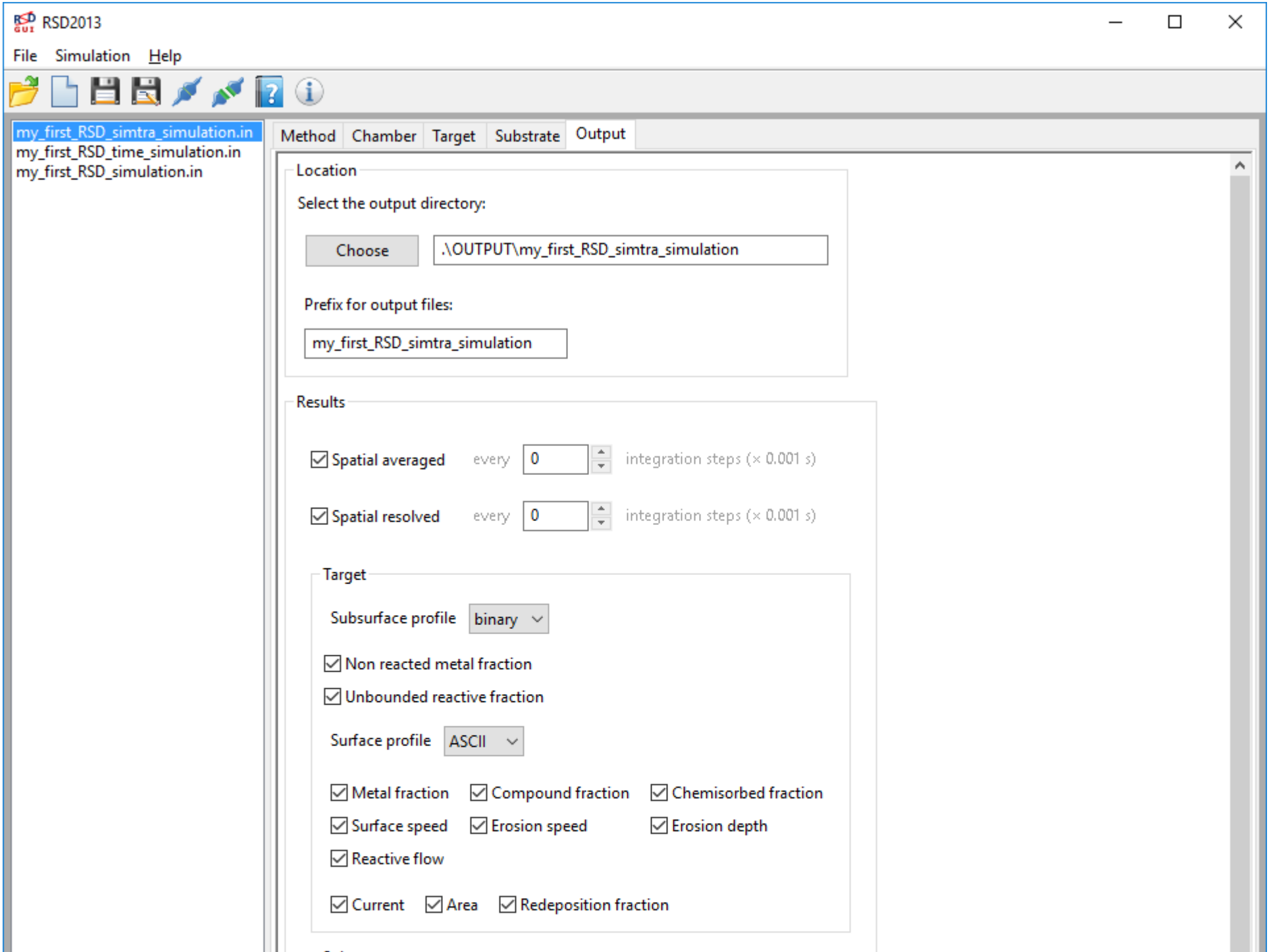
- `Area` (cm^2)
  The total surface area of all effective deposited substrates. Only applies if a `Uniform deposition` is chosen below.
- `Uniform redeposition`
  A spatial uniform deposition on all the substrates is considered.
  - `Fraction of sputtered flux`
    The fraction (between 0 and 1) of the total sputtered flux that is deposited on the considered substrate surfaces. The same fraction is used for both the sputtered metal as the sputtered reactive atoms. Editing this fraction changes in a conform way the redeposition fraction on the target, presented in `Target`> `Geometry`> `Redeposition`> `Uniform redeposition`> `Fraction of sputtered flux` or `Target`> `Geometry`> `Redeposition`> `Redeposition profile`> `Only profile with fraction`.
- `Deposition profile`
  A spatial resolved deposition profile is considered, typically based on SiMTra simulations.
  - `Manual input`
    Old style manner of including the redeposition distribution on the substrate based on a SiMTra deposition profile files. This way of including redeposition does not need the SiMTra input file, only the deposition profile files and the spatial areas they cover.
    - `Input file listing the deposition files:`
      An additional input file, the deposition listing file, lists all the SiMTra deposition profile files that contain the deposition distributions over the considered substrates besides their corresponding surface area. This file can be saved on the `Standard file location` or can freely be chosen by unchecking the box and editing the adjacent text field or using the `Choose` button. An already existing deposition listing file can also be loaded in the same way.
    - `Load deposition files`
      The locations of the SiMTra deposition profile files containing the deposition distributions can be looked up or the file locations can directly be given in line by line in the text field.

- `Collecting area`
  Each SiMTra deposition profile file defines a rectangular grid overlaying the considered surface. The area of this grid has to be provided and not the effective area of the considered surface.
- `Skip counts equal zero`
  Checking will exclude substrate cells in the overlaying grids that have a zero deposition fraction. These substrate cells are considered not real and will be assigned a -1 value in the RSD spatial resolved output files. This option is useful for example for a circular substrate surface which is covered by a rectangular grid. This results in unreal substrate cell in the grid corners.
- `Include rotation`
  Checking will need specification of `Rotation speed` for all the substrates listed. Only circular substrate surfaces are allowed to rotate here, other surfaces need a zero value.
  - `SiMTra configuration`
    This is the preferred way of including deposition distributions for the substrates. It is based on a SiMTra input file which should be specified in the text field under `Target`> `Metal particle M`> `SiMTra`.
    For the `Substrate`, `Object` list the SiMTra defined objects and `Surface` lists the composing surfaces of each `Object`. Non-editable properties of the `Object` and `Surface` are shown which can only be modified in the SiMTra GUI or the SiMTra input file
- `Object`
  The name of the object as defined in the SiMTra input file where the target surface is part of. The non-editable properties `Position` and `Orientation` of this object are listed. The symbol in front of the object name indicates if deposition profiles where saved during the SiMTra simulation and are included or not.
  ■ : all contained surfaces of this object have deposition profiles
  □ : all contained surfaces of this object have NO deposition profiles
  ◪ : some of the contained surfaces of this object have deposition profiles
- `Surface`
  The name of the surface as defined in the SiMTra input file for the selected The symbol in front of the surface name indicates if the deposition profile was saved during the SiMTra simulation and are included or not.
  ■ : surface has deposition profile
  □ : surface has NO deposition profile
  The non-editable properties `Type`, `Position` and `Orientation` within the local coordinate system, `Area` and `Grid resolution` are listed.
  Axial `Rotation` can be specified if the surface `Type` is a `circle`. Only a single SiMTra simulation is needed then. In the other case, it will not be visible or it states that it is `SiMTra specified` when `SiMTra`>`Use SiMTra deposition simulations`>`Enable movement` is selected and the possible movement of the surface will be accounted by SiMTra.
  - `Only fraction (uniform profile)`
    If checked, only the deposition fraction as simulated by SiMTra is used and a uniform deposition is considered.
  - `Only profile with fraction`
    If checked, only the relative depositoin profiles as simulated by SiMTra are used and scaled by the given deposition fraction. Editing this fraction changes in a conform way the redeposition fraction on the target, presented in `Target`> `Geometry`> `Redeposition`> `Uniform`

`redeposition`> `Fraction of sputtered flux` or `Target`> `Geometry`> `Redeposition`> `Redeposition profile`> `Only profile with fraction`.

Output

The window tab `Output` specifies which simulation results should be printed to a file, at which frequency and where to save these files.


RSD2013
File
Simulation
Help
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Location
Select the output directory:
Choose
.\OUTPUT\my_first_RSD_simtra_simulation
Prefix for output files:
my_first_RSD_simtra_simulation
Results
Spatial averaged
every
0
integration steps (× 0.001 s)
Spatial resolved
every
0
integration steps (× 0.001 s)
Target
Subsurface profile
binary
Non reacted metal fraction
Unbounded reactive fraction
Surface profile
ASCII
Metal fraction
Compound fraction
Chemisorbed fraction
Surface speed
Erosion speed
Erosion depth
Reactive flow
Current
Area
Redeposition fraction

Output window tab.

Location

- `Select the output directory`
  The directory where all RSD output files will be saved. The directory can be selected by `Choose` or by editing the text field. If the directory does not exist, the directory will be created. When a new RSD simulation is saved from an existing listed RSD simulation by using `Save as ...`, a new output directory is automaticly created with as name the name of the newly saved RSD main input file.
- `Prefix for output files:`
  In the text field a string prefix has to be specified which will be pre-appended to each RSD output file. When a new RSD simulation is saved by `Save as ...`, the prefix will automaticly assigned the name of the newly saved RSD main input file. Checking `Simulation`>`Auto prefix` will automaticly attribute a number to the prefix field and gray out this field for all simulations listed in the simulation list window.

Results

By checking the boxes, desired simulation output can be selected to be printed out in files. 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.
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.

- `Spatial averaged`
  Checked will always create an output file with the suffix `hyst_steady.out`. This output file contains the simulated system variables under steady state conditions. If the `Time evolution method` is chosen an additional output file with the suffix `hyst_time.out` is created. This output file contains the simulated system variables as a function of time. The used time interval for printing out results can be specified by a multiple of the intergration `Time step`. If this multiple is set 0 than only at the end of every simulation step (= a specific set of operation conditions), the results will be printed out. Additional info about these two output files can be found in the section Spatial averaged.
- `Spatial resolved`
  Checking this box will only be possible when `Multi-cell` for the `Target` and/or the `Deposition profile` for the `Substrate` is chosen. In this case the check boxes under `Target` and `Substrate` will become available. The used time interval for printing out results can be specified by a multiple of the intergration `Time step`. If this multiple is set 0 than only at the end of every simulation step (= a specific set of operation conditions), the results will be printed out.
  - `Target`
    - `Subsurface profile` **[RSD only]**
      Spatial 1-dimensional data if a `One-cell` target is chosen. Spatial 2 or 3-dimensional data if a `Multi-cell` target is chosen.

- `Non reacted metal fraction`
  The relative metal concentration n_M/n_0 in the target subsurface that is not chemical reacted with the implanted reactive gas atoms.
   The relative reacted metal concentration is simply the complement $1-n_M/n_0$.
- `Unbounded reactive fraction`
  The relative reactive gas concentration n_R/n_0 in the target subsurface that is not bounded to the metal atoms.
- `Surface profile`
  Spatial 2-dimensional data which is available if a `Multi-cell` target is chosen.
- `Metal fraction`
  The metal M atom fraction θ_m at the target surface where no reactive gas atoms are bounded on.
- `Compound fraction` **[RSD only]**
  The atom MR_z fraction θ_r at the target surface where z reactive gas atoms are chemical bounded on.
- `Chemisorbed fraction`
  The atom MR_z fraction θ_c at the target surface where z reactive gas atoms are chemisorbed on.
- `Surface speed` (cm s^{-1})
  The effective speed v_s of the target surface.
- `Erosion speed` (cm s^{-1})
  The erosion speed v_e of the target surface if no redeposition is considered.
- `Erosion depth` (cm)
  The deepening of the target by the effective surface speed. Only applicalbe if the `Time evolution method` is chosen.
- `Reactive flow` (sccm)
  The reactive molecular gas flow Q_t) gettered by the target.
- `Ion current` (A)
  The ion current I_{ion} that flows through the target surface.
- `Area` (cm^2)
  The area A_t of the target surface.
- `Redeposition fraction` (cm^{-2}) **[RSD only]**
  The redeposition fraction ε_t per unit of area on the target.

o `Substrate`

- `Surface profile`
  Spatial 2-dimensional data which is available if a `Deposition profile` for the `Substrate` is chosen.
- `Compound fraction`
  The atom MR_z fraction θ_s at the substrate surface where z reactive gas atoms are chemical bounded on.
- `Reactive flow` (sccm)
  The reactive molecular gas flows Q_s) gettered by the substrate cells.
- `Area` (cm^2)
  The surface areas A_t of the substrate cells.

- `Deposition fraction` (cm^{-2})
  The deposition fractions ε_S per unit of area on the substrate cells.
  - `Input file with the results specifications`
    The selection of which results are printed out to files and in which format are saved in an additional input file, the result specification file. This file can be saved on the `Standard file location` or can freely be chosen by unchecking the box and editing the adjacent text field or using the `Choose` button. An already existing result specification file can also be loaded in the same way.

Simulation list

The simulation list window lists the loaded or created simulation inputs. A simulation in the list is represented by the file name 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.

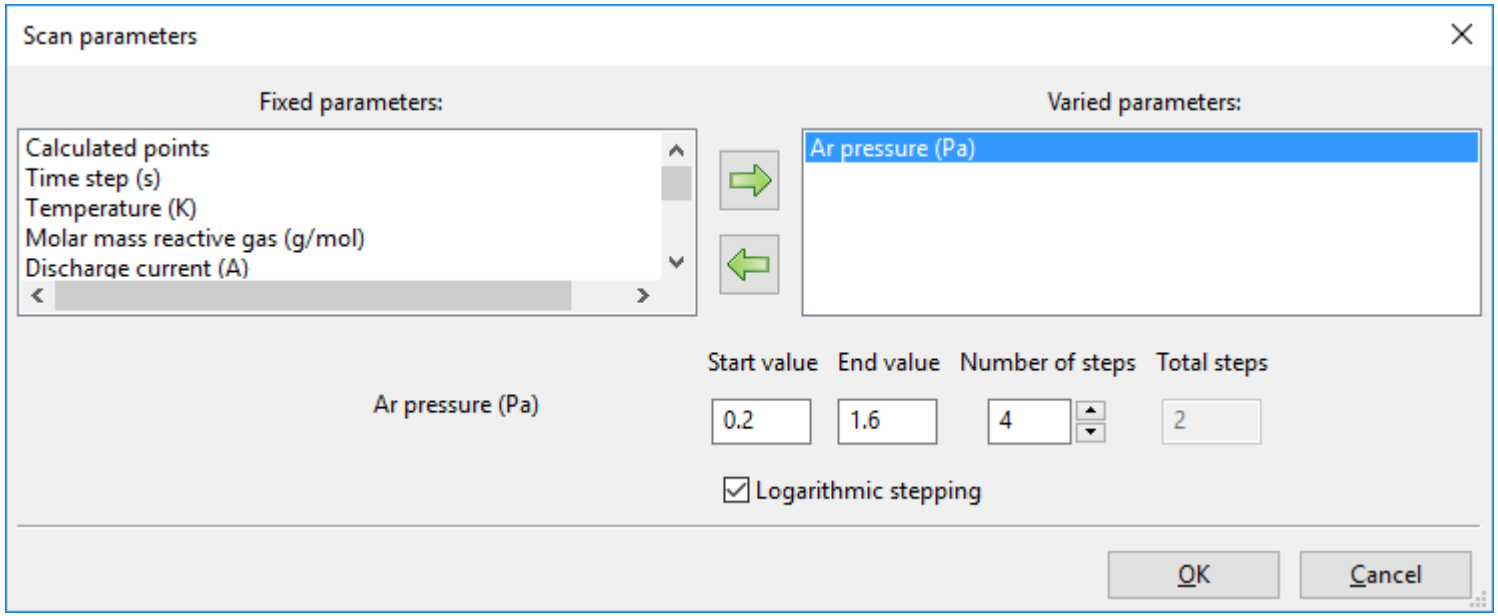
The simulation input which is current in scope is blue highlighted in the simulation list window. Selecting another simulation in the list will automaticly save the made changes in the previous simulation input.

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

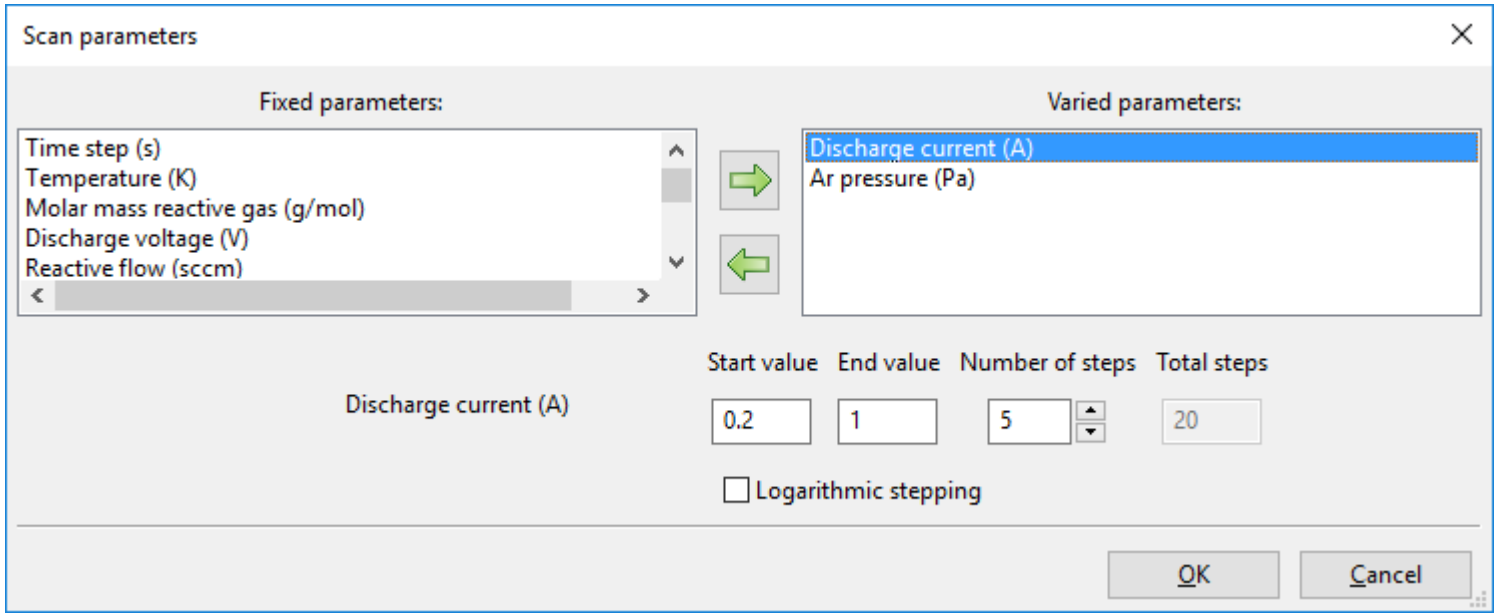
- `Delete`
  Key stroke that removes the selected simulations from the list.
   The input files are NOT removed from your disk, only from the simulation list window.
- `Simulation`>`Run selected` 
  Sequentially run the selected simulations.

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

- `Scan`
  Allows to automaticly generate a series of simulations where one or more parameters is varied over a predefined range.



Scan window, one varied parameter.



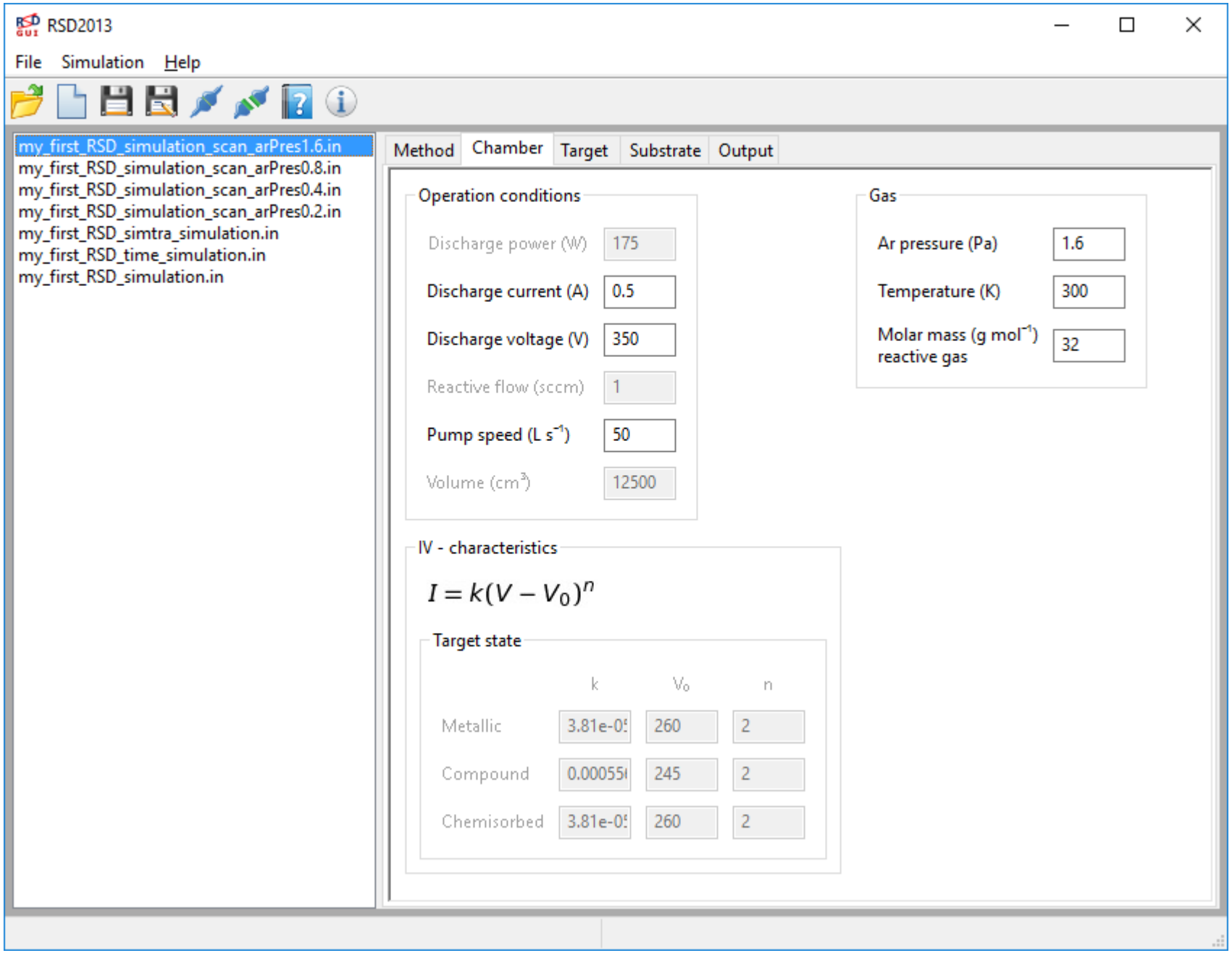
Scan window, two varied parameter.

Scan

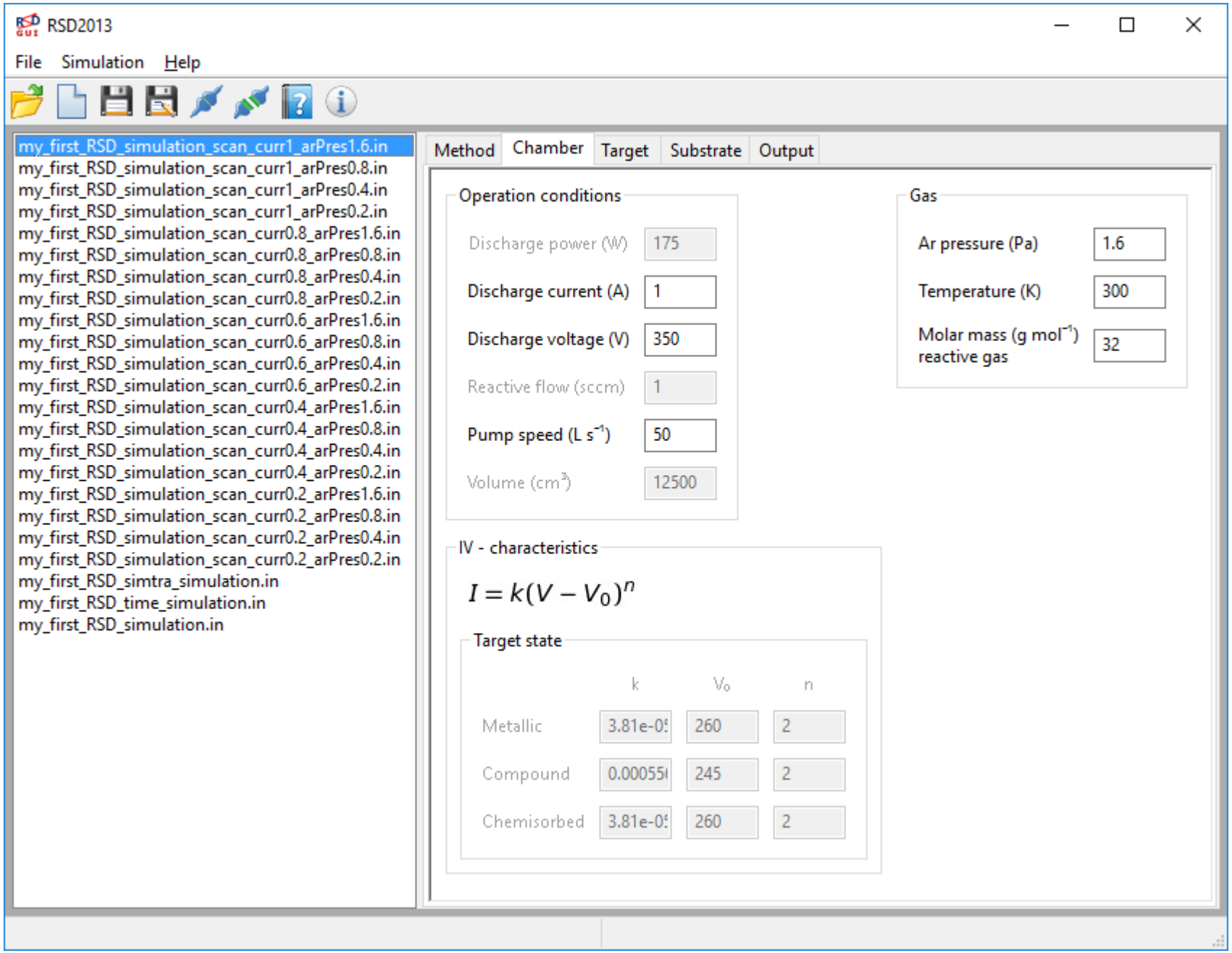
The `Scan` action allows to do a multiple parameter scan. This action is executed on a selected simulation input from the simulation list window. Most parameters of the simulation input can then be varied. For each parameter combination, a new main input file will be generated and as such be inserted as a new item in the simulation list window.
Selecting this `Scan` action for an item in the window list pops up the scan window. Two lists are defined:

- `Fixed parameters`
  It lists the parameters that can been chosen to do a parameter scan for.
- `Varied parameters`
  Initial an empty list where items of the `Fixed parameters` list can be placed in by the right arrow and put back by the left arrow. 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`
    Start value (lower limit) of the selected parameter in the `Varied parameters` list.

- `End value`
  End value (upper limit) of the selected parameter in the `Varied parameters` list.
- `Number of steps`
  Number of parameter values that will be accessed for the selected parameter in `Varied parameters` defined by `Start value` and `End value`, including (at least) these lower and upper limit.
- `Total steps`
  Total number of simulations created based on all the parameter variations. Non-editable field.
- `Logarithmic stepping`
  Checking will logarithmicly spread the values for a selected parameter over its range where the default is linearly.
  Pressing `Ok` will generate the simulation inputs and add them to the simulation list window. 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 the value of the scanned parameter.
   The generated main input files will NOT have an own copy of the referenced additional input files.


RSD2013
File
Simulation
Help
my_first_RSD_simulation_scan_arPres1.6.in
my_first_RSD_simulation_scan_arPres0.8.in
my_first_RSD_simulation_scan_arPres0.4.in
my_first_RSD_simulation_scan_arPres0.2.in
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Operation conditions
Discharge power (W)
175
Discharge current (A)
0.5
Discharge voltage (V)
350
Reactive flow (sccm)
1
Pump speed (L s-1)
50
Volume (cm3)
12500
Gas
Ar pressure (Pa)
1.6
Temperature (K)
300
Molar mass (g mol-1) reactive gas
32
IV - characteristics
$I = k(V - V_0)^n$
Target state
k
V0
n
Metallic
3.81e-05
260
2
Compound
0.000551
245
2
Chemisorbed
3.81e-05
260
2

Simulation list window with one varied parameter.


RSD2013
File
Simulation
Help
my_first_RSD_simulation_scan_curr1_arPres1.6.in
my_first_RSD_simulation_scan_curr1_arPres0.8.in
my_first_RSD_simulation_scan_curr1_arPres0.4.in
my_first_RSD_simulation_scan_curr1_arPres0.2.in
my_first_RSD_simulation_scan_curr0.8_arPres1.6.in
my_first_RSD_simulation_scan_curr0.8_arPres0.8.in
my_first_RSD_simulation_scan_curr0.8_arPres0.4.in
my_first_RSD_simulation_scan_curr0.8_arPres0.2.in
my_first_RSD_simulation_scan_curr0.6_arPres1.6.in
my_first_RSD_simulation_scan_curr0.6_arPres0.8.in
my_first_RSD_simulation_scan_curr0.6_arPres0.4.in
my_first_RSD_simulation_scan_curr0.6_arPres0.2.in
my_first_RSD_simulation_scan_curr0.4_arPres1.6.in
my_first_RSD_simulation_scan_curr0.4_arPres0.8.in
my_first_RSD_simulation_scan_curr0.4_arPres0.4.in
my_first_RSD_simulation_scan_curr0.4_arPres0.2.in
my_first_RSD_simulation_scan_curr0.2_arPres1.6.in
my_first_RSD_simulation_scan_curr0.2_arPres0.8.in
my_first_RSD_simulation_scan_curr0.2_arPres0.4.in
my_first_RSD_simulation_scan_curr0.2_arPres0.2.in
my_first_RSD_simtra_simulation.in
my_first_RSD_time_simulation.in
my_first_RSD_simulation.in
Method
Chamber
Target
Substrate
Output
Operation conditions
Discharge power (W)
175
Discharge current (A)
1
Discharge voltage (V)
350
Reactive flow (sccm)
1
Pump speed (L s-1)
50
Volume (cm3)
12500
Gas
Ar pressure (Pa)
1.6
Temperature (K)
300
Molar mass (g mol-1) reactive gas
32
IV - characteristics
I = k(V − V0)n
Target state
k
V0
n
Metallic
3.81e-05
260
2
Compound
0.000551
245
2
Chemisorbed
3.81e-05
260
2

Simulation list window 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 the Command Prompt if it is provided with the absolute path of a main input file or its 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 additional 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 additional input files.
- The additional input files define more specific input data and options for a simulation or further path references to additional 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 input file

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.

my_first_RSD_simtra_simulation.in - Notepad

File Edit Format View Help

```
#
# Main input file for RSD2013_v3
#
##################################
#
# row 1 : Pressure of the sputter gas (e.g. Ar) [Pa]
# row 2 : Discharge current [A=C/s]
# row 2a : Discharge voltage [V]
# row 2b : Discharge power [W]
# row 3 : Molar mass of reactive gas (e.g. O2) [g/mol]
# row 3a : Reactive gas flow [sccm]
# row 4 : Molar mass of target material (e.g. Al) [g/mol]
# row 5 : Mass density of target material (e.g. Al) [g/cm^3]
# row 5a : Specifies if dilution of the sputter yield due to implanted non-bounded reactive ions is included or not
#                  by the following keywords:
#                - "dilution" : dilution of the sputter yield is included
#                - "NA" : no dilution of the sputter yield is included
# row 5b :      Sputter yield Y_R [#R particle/ion] of the unbounded implanted reactive gas atom specified by a linear
#               Y_R = b + a * V with the parameters b (first parameter) and a (second parameter) (e.g. 1. 0)
#
# row 6 :       Sputter yield Ym [#M particle/ion] of the metal fraction specified by a linear function of the discharg
#               Ym = b + a * V with the parameters b (first parameter) and a (second parameter) (e.g. 0.5 0)
#
# row 6a :      Secondary elektron emission yield of the metal fraction [#e-/ion]
#
# row 6b : Current-voltage (IV) characteristic of the target in the metallic state by the relation I = k(V-V_0)^n
#                with the parameters k (first parameter), V_0 (second parameter) and n (third parameter) (e.g. 3.81e-5
#
```

Comment section of main input file.

my_first_RSD_simtra_simulation.in - Notepad

File Edit Format View Help

```
# row 44 : In case of the steady state solution (row31), it specifies the range of the partial reactive pressure (e.g. (
#               its maximum, minimum and the partitioning of the interval with the keywords:
#                - "lin" when a linear partitioning of the interval is wanted
#                - "log" when a logarithmic partitioning of the interval is wanted
#                In case of the time solution (row31), it specifies the output periode as an integer times the integrat
#                - "0" when only the results at steady state should be printed
#
# row 45 : File location of file that specifies which output should be generated
#
# row 46 : Specifies which model you want to use for the simulation with one of the following keywords:
#                - "RSD2013" to use the RSD2013 model with chemisorption and implantation as reaction mechanism
#                - "Berg" to use the Berg model with chemisorption as reaction mechanism
row001  0.4
row002  0.5
row002a 350
row002b 175
row003  32
row003a 1
row004  26.98
row005  2.702
row005a no_dilution
row005b 0 0
row006  -0.111 0.00191
row006a 0.1
row006b 3.81e-05 260 2
row007  0.005 6e-05
row007a 0
row007b 3.81e-05 260 2
```

Input section of main input file.

The structure of the file is as follows. It starts with a comment section where every line starting with `#` is considered as a comment line and is ignored. After this comment section, each 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.

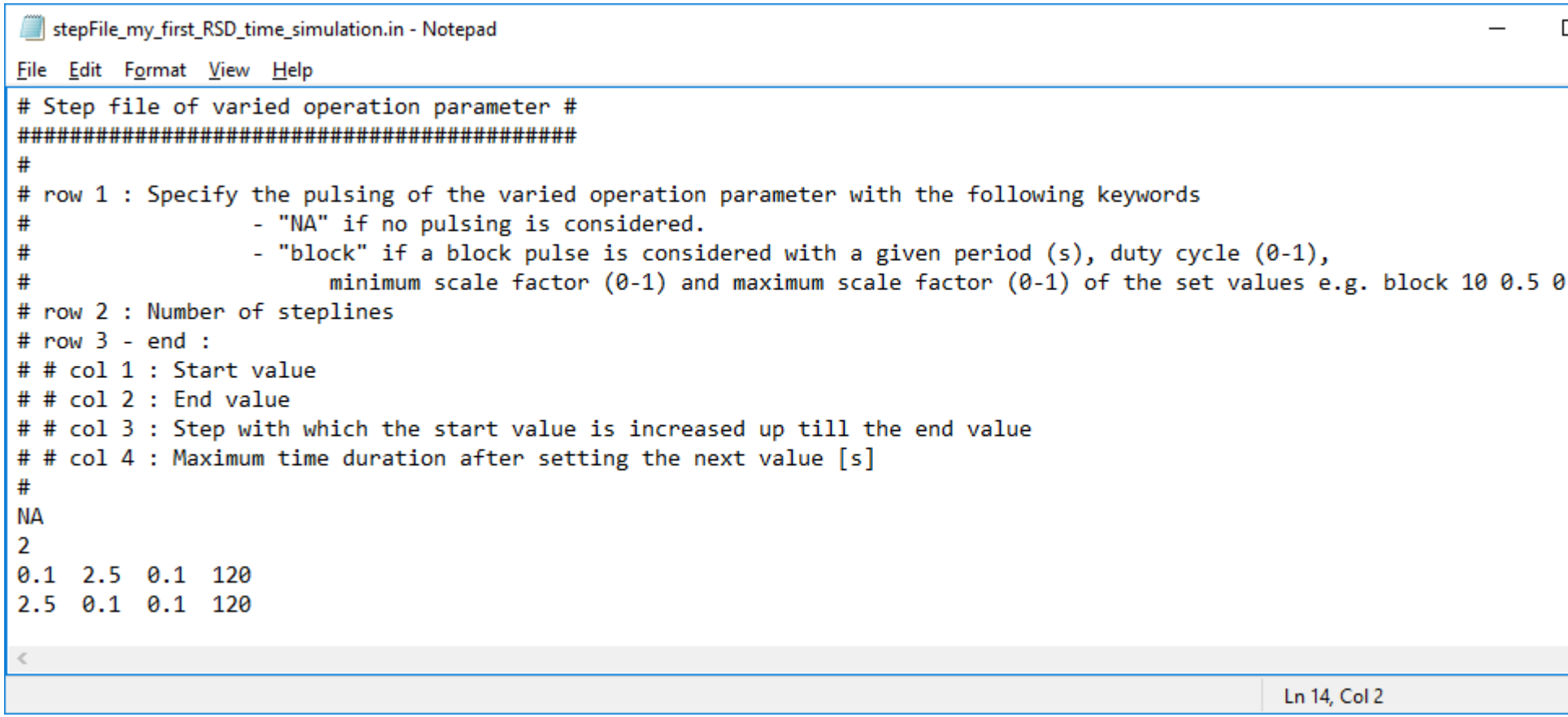

Almost no input restrictions apply in the GUI, and no validity check at the start of a simulation run is performed. Give valid input values are up to the responsibility of the user.

Additional input files

The additional input files are all other input files than the main input file. The main input file contains references to these additional input files, but these additional input files can also contain further references to other additional input files. Several types of additional input files the RSD2013 software possibly needs and/or creates are given below.

Step file

The step file can be created or modified under `Method`> `Solution method`> `Time evolution method`> `Step file`.



Step file.

The step file defines the evolution of the `Varied operation parameter(s)` for the `Time evolution method`. This input file can be edited or loaded in the window tab `Method`>`Stepfile` when choosing the `Time evolution method`. The step file is a text based file which consist out of numerical text lines. After an optional comment section (lines starting with `#`), the pulsing of the `Varied operation parameter(s)` can be specified as no pulsing `NA` or block pulsing `block`. The second non-comment line should contain the number of value ranges (or numerical text lines) that are specified next. Each consecutive line defines then a range over which the `Varied operation parameter(s)` may be varied. The first entry of such a line defines the start value, the second entry the end value, the third entry the step with which the start value is stepwise increased until it reaches the end value. The last entry is the maximum time the given `Varied operation parameter(s)` may be set, depending on the chosen options for the parameter stepping.

Current profile file

The current profile file can be loaded under `Target`> `Geometry`> `Multi-cell`> `Current profile`.
The current profile file 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 has not be particularly normalized.

- `circular`
  An axial symmetric profile is assumed where as such only an 1-dimensional radial profile has to be specified. The first entry of each line is the radial distance, the second entry is the value of the profile at that position. Only the relative radial distance is importants as the profile will be scaled on the target `Area`.

racetrack_Al_2inch.in - Notepad

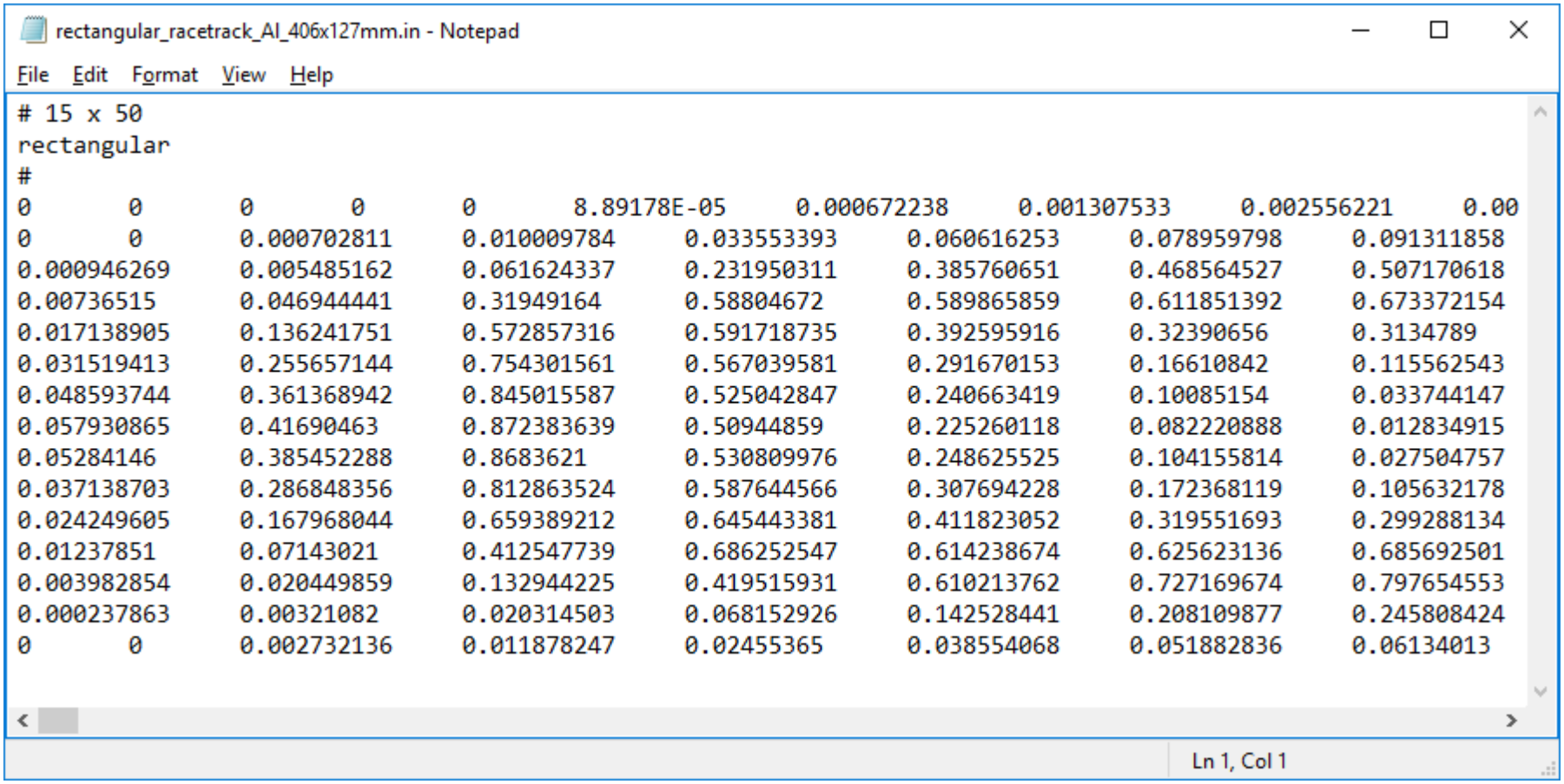
File Edit Format View Help

```
#
# Sputter eroded 2inch Al target for rotating disk (by Roeland Schelfhout)
#
circular
#
0       0
0.559524793     0.00792314
1.08427686      0.005618382
1.590061983     0.015853676
2.545785124     0.025150865
3.180123967     0.022364792
3.679586777     0.020171107
4.238057851     0.031213062
4.836570248     0.080487457
5.016756198     0.13263724
5.362376033     0.190288798
5.92822314      0.265658218
6.452975207     0.355741003
6.653181818     0.426487976
7.145268595     0.555122535
7.644731405     0.677496324
7.996673554     0.788061289
8.303305785     0.87183564
```

Ln 1, Col 1

Circular current profile file.

- `rectangular`
  A 2-dimensional rectangular profile has to be specified as 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 matrix elements represents the relative ion current to the target cell.



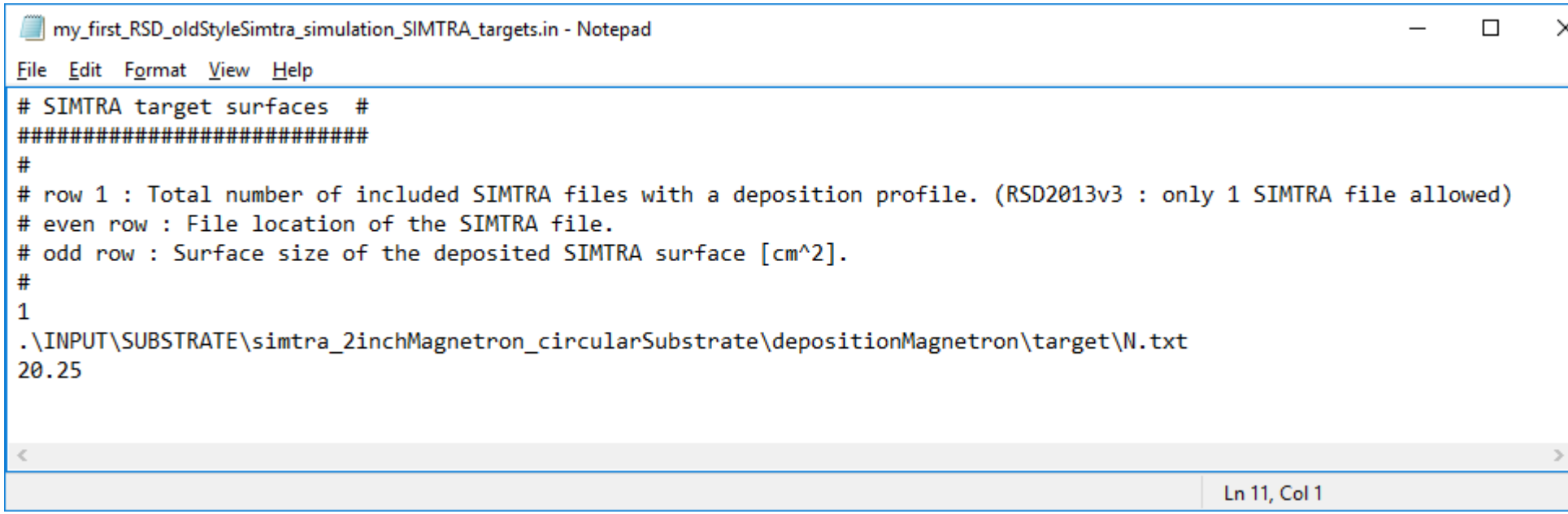
Rectangular current profile file.

SiMTra input file

The SiMTra input file can be loaded and modified under `Target`>`Metal particle M`> `SiMTra`.
The SiMTra input file should be a valid input file for the SiMTra version 2.2 For details about this file, check the SiMTra documentation.

(Re)deposition listing file

The (re)deposition listing file can be loaded and/or assigned under `Target`> `Geometry`> `Redeposition`> `Manual input`> `Input file listing the deposition files` for the target and under `Substrate`> `Geometry`](#SubstrateGeometry)> `Deposition profile`> `Manual input`> `Input file listing the deposition files` for the substrates.



Redeposition listing file.

my_first_RSD_oldStyleSimtra_simulation_SIMTRA_substrates.in - Notepad

File Edit Format View Help

```
# SIMTRA substrate surfaces  #
##############################
#
# row 1 : Total number of included SIMTRA files with a deposition profile.
# even row : File location of the SIMTRA file.
# odd row : Surface size of the deposited SIMTRA surface [cm^2].
#
9
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionChamber\xmax\N.txt
900
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionChamber\xmin\N.txt
900
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionChamber\ymax\N.txt
900
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionChamber\ymin\N.txt
900
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionChamber\zmax\N.txt
900
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionChamber\zmin\N.txt
900
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionDummyObjects\table\leftDisk\N.txt
100
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionDummyObjects\table\rightDisk\N.txt
100
.\INPUT\SUBSTRATE\simtra_2inchMagnetron_circularSubstrate\depositionDummyObjects\table\mantle\N.txt
15.7
```

Ln 15, Col 87

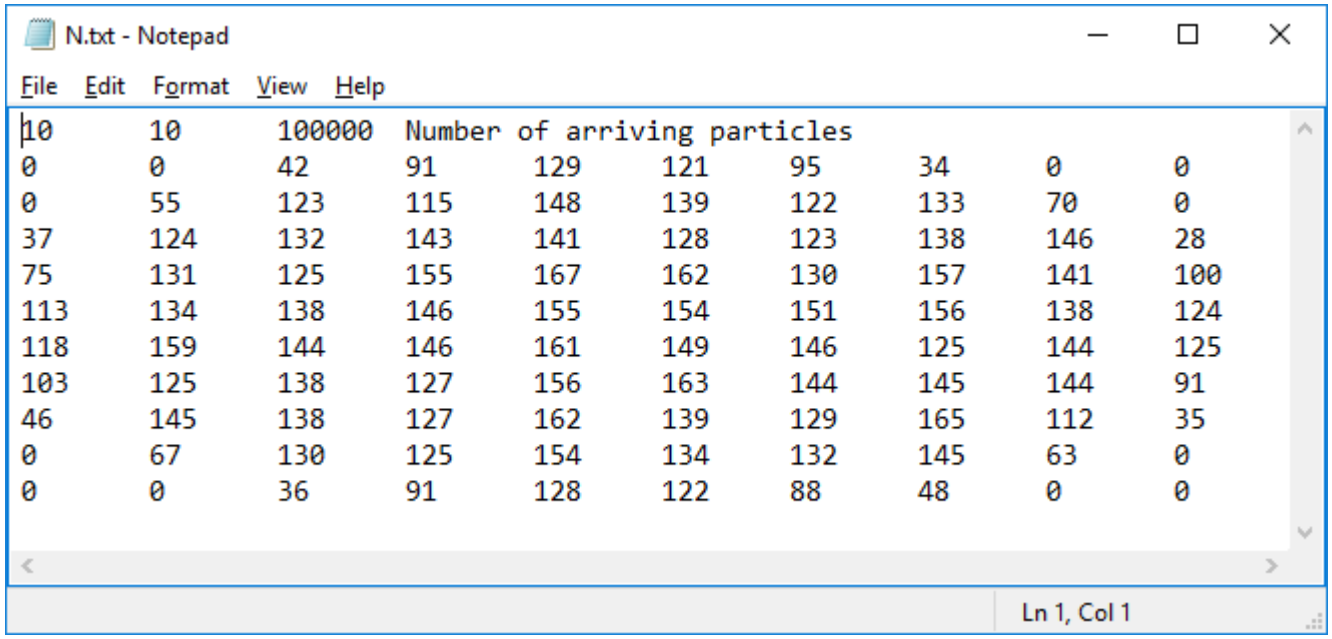
Deposition listing file.

Only needed if the old style of including deposition distributions is used (`Manual input`). The preferred way is the loading a SiMTra input file.
The file lists the deposition profile files for the target (only one) or for the substrate (multiple possible). Its structure is as follows: the first non-comment line of the file gives the number of included (re)deposition profile files. Each following couple of lines represent the full path or relative path of the deposition profile file, while the second line contains the area which corresponds with the deposition profile. This area should take into account the full rectangular matrix of the profile, also when there are (ignored) zero elements (`Skip counts equal zero`).

(Re)deposition profile file

A single redeposition profile file can be loaded under `Target`> `Geometry`> `Redeposition`> `Manual input`> `Load deposition files` for the target and multiple deposition files can be loaded under `Substrate`> `Geometry`> `Deposition profile`> `Manual input`> `Load deposition files` for the substrates.

Only needed to be specified if the old style of including deposition distributions is used (`Manual input`). The preferred way is the loading a SiMTra input file



Deposition file.

A (re)deposition profile file defines the relative number of sputtered particles (atoms) that is deposited on a surface. Such file is text based and matrix structured conform a deposition file from SIIMTra. The first two entries on the first line define respectively the number of rows and columns of the matrix. The rest of the line is ignored. All following lines define the matrix with integers.

Result specification file

The result specification file can be specified or loaded under `Output`> `Results`> `Input file with the results specifications`.
The file with the results specifications determines which output will be generated when a simulation is executed. The text file structure closely resemblance the window tab `Output`.
With each kind of output, a keyword is linked. When this keyword is not preceded by `x`, `o` or `v`, this output is not printed to file. The `x` is used for a checkbox, the `o` for a radiobutton and `v` for a choice in a roll-down list.

my_first_RSD_simtra_simulation_OutputSpecs.in - Notepad

File Edit Format View Help

```
# File with output specifications
########################
#
#  The specification of the output options in resemblance with the GUI
#               'x'     Check a checkbox (apply this option)
#               'o'     Check a radiobutton (apply this chosen option)
#               'v'     Choose this item out of the list (apply this chosen option)
#               ' '     Do not apply
#
#       Hierarchy
#                                       Head caterogy
#               -                       First subcategory
#               --              Second subcategory
#               ---     Third subcategory
#
########################
x       Spatial averaged
x       Spatial resolved
                -Target bulk ascii
v       -Target bulk binary
                --Metal fraction
                --Reactive fraction
v       -Target surface ascii
                -Target surface binary
x       --ThetaM
                --ThetaR
                --ThetaC
                --Surface speed
                --Erosion speed
                --Erosion depth
                --Target flow
                --Current
                --Area
                --Redeposition
                -Substrate surface ascii
v       -Substrate surface binary
x       --ThetaS
```

Result specification file.

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.

The frequency of printing out results as a multiple of the `Time step`, is saved in the main input file.

Output files

Output files always have the extension `.out`. Which output files are produced, is determined by the result 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 for output files` and ends with an unique keyword string.

Spatial averaged

Two output files may correspond with the `Spatial averaged` option. For the `Steady state method`, only an output file with suffix `hyst_steady.out` is produced. Each column in this file states the following steady state variables

1. Q_r : flow of reactive gas introduced in the vacuum chamber
2. p_r : partial 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_m,ss : spatial averaged metal fraction at the target surface/subsurface interface
8. n_R/n0 : relative concentration of non-reacted implanted reactive gas atoms at the target surface/subsurface interface
9. Q_p : reactive gas flow pumped away by the vacuum pump
10. Q_s : reactive gas flow consumed by compound formation on the substrate
11. Q_t : reactive gas flow consumed (> 0) or released (< 0) by the target
12. V : discharge voltage
13. I : discharge current
14. I_ion : ion current to the target
15. S : pumping speed of the vacuum pump

my_first_RSD_time_simulation_hyst_time.out - Notepad

File Edit Format View Help

# Q_r[sccm](1)	p_r[Pa](2)	theta_s(3)	theta_m(4)	theta_c(5)	theta_r(6)	theta_m,ss(7)	n_R/n0(8)
0.1	0	0	1	0	0	1	0
0.1	0.000158423	0.00311844	0.998496	0.000945699	0.000558172	0.999846	0.00154334
0.1	0.000159465	0.00634743	0.997766	0.000995046	0.00123925	0.999835	0.00163878
0.1	0.000159934	0.00927254	0.997497	0.000999034	0.00150392	0.999834	0.0016464
0.1	0.00016035	0.0119175	0.997395	0.0010016	0.00160344	0.999833	0.00165104
0.1	0.000160726	0.0143082	0.997354	0.00100396	0.00164231	0.999833	0.00165513
0.1	0.000161068	0.0164687	0.997335	0.00100614	0.00165889	0.999833	0.00165881
0.1	0.000161378	0.0184211	0.997325	0.00100811	0.00166715	0.999832	0.00166215
0.1	0.00016166	0.0201854	0.997318	0.00100991	0.00167218	0.999832	0.00166517
0.1	0.000161915	0.0217797	0.997313	0.00101154	0.00167585	0.999832	0.00166791
0.1	0.000162146	0.0232204	0.997308	0.00101302	0.00167885	0.999831	0.00167039
0.1	0.000162355	0.0245222	0.997304	0.00101436	0.00168146	0.999831	0.00167264
0.1	0.000162545	0.0256986	0.997301	0.00101558	0.00168377	0.999831	0.00167468
0.1	0.000162717	0.0267617	0.997297	0.00101668	0.00168586	0.999831	0.00167653
0.1	0.000162873	0.0277223	0.997295	0.00101768	0.00168774	0.999831	0.0016782
0.1	0.000163014	0.0285903	0.997292	0.00101858	0.00168944	0.99983	0.00167972
0.1	0.000163141	0.0293747	0.99729	0.00101939	0.00169098	0.99983	0.00168109
0.1	0.000163257	0.0300835	0.997287	0.00102013	0.00169237	0.99983	0.00168233
0.1	0.000163361	0.030724	0.997286	0.0010208	0.00169363	0.99983	0.00168345
0.1	0.000163455	0.0313028	0.997284	0.00102141	0.00169478	0.99983	0.00168447
0.1	0.000163541	0.0318258	0.997282	0.00102195	0.00169581	0.99983	0.00168538
0.1	0.000163618	0.0322984	0.997281	0.00102245	0.00169674	0.99983	0.00168622

Output file `hyst_time.out`.

For the `Time evolution method`, this file contains the values of the variables at the end of every `Varied operation parameter(s)` step. A second output file is also generated with suffix `hyst_time.out`. This file contains the same variables as above, but adds as 12th column the time elapsed in the simulation.

1. t : time in the simulation

The spatial averaged variables correspond with these time stamps where the frequency is specified as a multiple of the `Time step`.

 The `spatial averaged` values are in fact weighted by the `Current profile`.

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 profile (2-D)

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 `Output`> `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.

 If a substrate surface (only a `Circle`) is specified to axial rotate at a given speed within RSD, not if `Enable movement` is selected, the output matrix is a polar representation of the surface with the rows as the radial and the columns as azimuthal dimension.
The data of the surface is saved at every steady state point if 0 is specified for `Spatial resolved` or at the specified multiples of the `Time step` The row numbering is restarted after every print out. A value of -1 means that this surface cell is not considered in the simulation.
For the `Spatial resolved` substrate:
- `Substrate`> `Geometry`> `Deposition profile`> `Manual input` :
The output file names are suffixed with the order number as they occur in the deposition listing file.
- `Substrate`> `Geometry`> `Deposition profile`> `SiMTra configuration` :
The same directory structure as the SiMTra output for the different `Object` and `Surface` is constructed with the `Object` name and `Surface` name appended to the file names.

Subsurface profile (3-D)

Subsurface resolved output can be generated for the target when choosing a current profile. A table listing the different variables which can be resolved for the subsurface is given under `Results`.
The format of the file is as follows. The first entry of the first line is 100, 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 *μ* + 3*σ* for a Gaussian profile or the `Depth` for a uniform 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 values for the corresponding surface cell.
The data of the surface is saved at every steady state point if 0 is specified for `Spatial resolved` or at the specified multiples of the `Time step` The row numbering is restarted after every print out. A value of -1 means that this surface cell is not considered in the simulation.

End remark

I would be grateful for any comment, suggestion for improvement, mistake or typo occurring in this documentation or software. Feel encouraged to contact us at koen.strijckmans@ugent.be (or diederik.depla@ugent.be).