VIRTUAL COATER™

<u>MakeProcess Manual for version 4.8</u>

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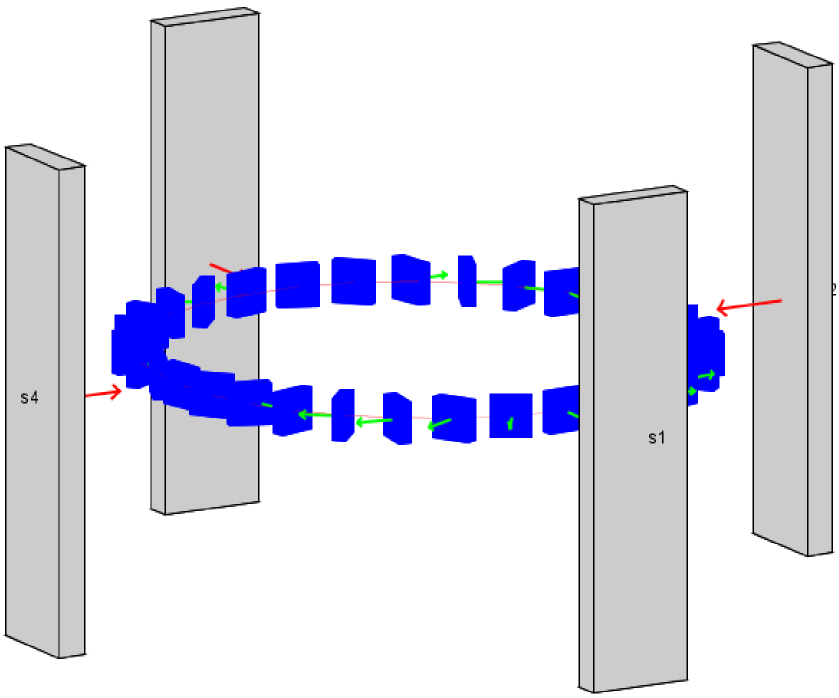

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Table of Contents

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1. Introdiction

Make Process is a tool which enables creating a digital twin of a user's coater. With the help of Make Process one can calculate parameters of depositing material flows from a several sources to a moving or fixed substrate. Make Process calculates a relative amount of material deposited from any source to a substrate at a given position, as well as energy and angular distributions of atoms arriving from these sources to the substrate. Afterwards, one can generate simulations of film growth on a moving or fixed substrate which use all the data (namely, relative amount of deposited material, energy and angular distributions) obtained by means of Make Process as input parameters.

Make Process considers gas pressure in deposition chamber, positions of sources and substrate, their mutual orientations.

2. User Interface

The main window of Make Process has 4 tabs, Parameters, Results, Log, and Stacks, see Figure 1.

The Parameters tab has three main windows where a user can set up the simulations. In the left window one can set up sources of depositing materials as well as substrate motion. In the bottom right window "General parameters" a user can set up several parameters of simulations, such as duration of a process, number of deposited atoms etc. In the upper right window, a user can see a visualization of his process: position and orientation of the sources, trajectory of the substrate.

The Result tab displays simulations results, such as angular and energy distributions of depositing particles as well as time dependent fluxes from each source to a substrate.

The Log tab is intended to display simulation details.

Finally, the Stack tab is used to setup simulation of deposition in a multi-chamber coater.

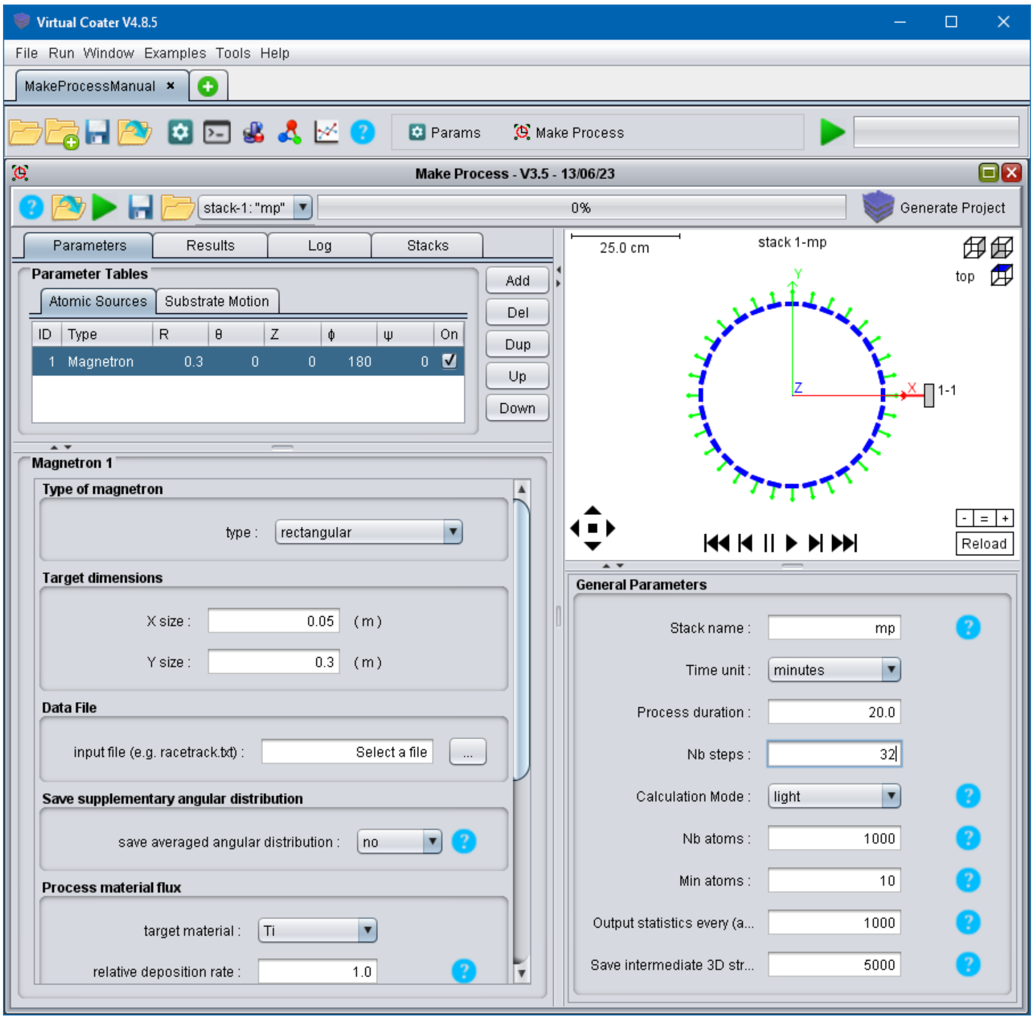

Figure 1. Main interface of Make Process plug-in.

1.1. Process viewer

This window represents a schematic view of the coater. One can see positions and orientations of sources and a substrate in motion. Using arrows one can animate substrate motion. Also, it is possible to zoom in and out, change orientation and move the view of the virtual coater.

1.2. Sources

To setup a source it is necessary to go through the following steps:

- Set up the position and orientation of the source,
- Define if the target is rectangular or circular,
- And define target dimension,

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- Afterwards for the case of "full" simulation mode (see below) it is necessary to specify the racetrack datafile,
- Specify target materials, relative deposition rate for the case when several sources are in use, stoichiometry index for the case of reactive deposition,
- Specify if the flux is constant or variable,
    - In case of variable flux one can set up parameters of flux variation,
- Specify working pressure in the coater,
- Finally, one should specify the energy range of the interest for of energy distribution of depositing particles.

1.3. Substrate Movement

In the Substrate motion tab one can set up the trajectory of the substrate, see Figure 2. There are several types of substrate motion: Linear translation, rotation, oscillation, tilting, in addition one can set up the trajectory by means of a data file. It is possible to combine several substrate motions by superimposing one motion onto the other. This makes it possible to set up the substrate motion very flexibly.

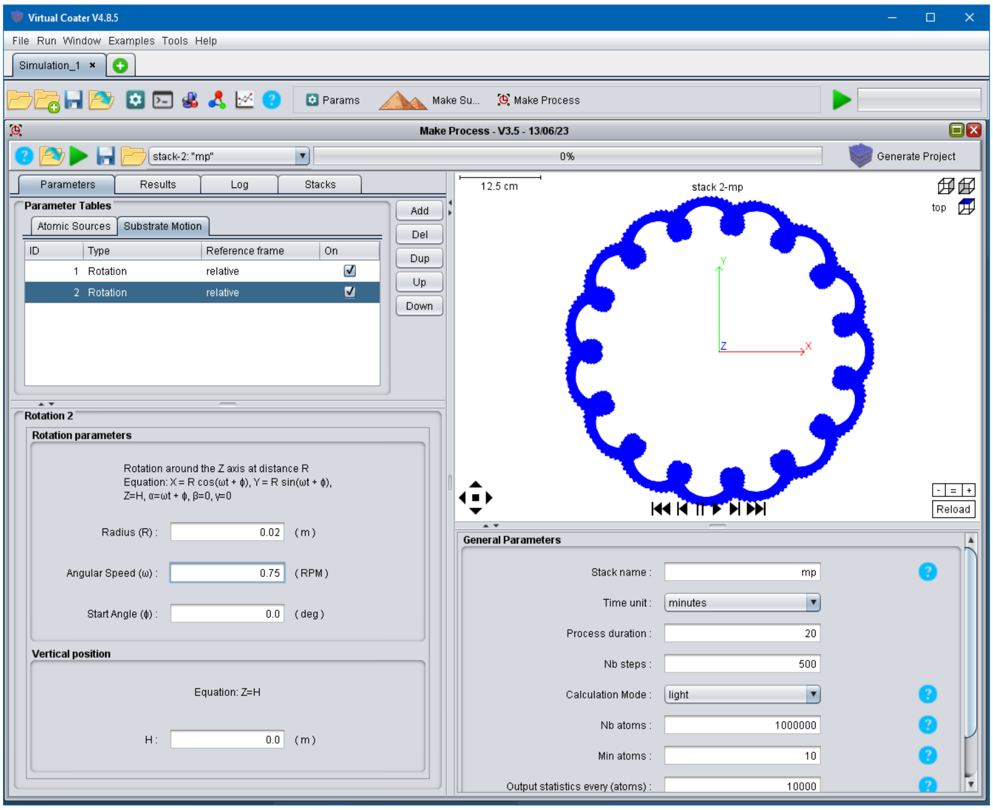

Figure 2. An example of substrate motion setup

One of a common example of such motion combination is the combination of two or more rotation, see Figure 2, that enables simulation of a coater with two or three folded rotations.

1.4. General Parameters

In this window one should set up the general parameters of the simulations:

- Mane of the simulation stack,
- The duration of the deposition process,
- Number of steps, in which the whole substrate motion is discretized. The higher the number of steps, the higher the accuracy, but the simulation time also increases with the number of steps. Thus, one can find an optimal value for this parameter.
- Calculation mode may be light or full. In a light mode target racetracks are not taken into account. That makes the simulation fast but not too accurate. In the full mode target racetracks are considered, thus simulation in this mode is more accurate.
- Next parameters specify data for film growth simulations:
    - "Nb atoms" specifies the total number of atoms that are deposited in a film growth simulation.
    - "Min atoms" is the minimal number of atoms which are considered for film growth simulations. If the calculated number of atoms to deposit at a given substrate position is less than this number, it is supposed that there is no deposition at that position.
    - "Output statistics" specify how often statistics are saved.
    - Finally, last value specify how often intermediate screenshots of growing film are saved.

3. Stages

The Stacks tab enables a user to do simulations of multi-chamber/compartment coaters. Each stack represents one chamber of a coater. Thus, one can set up each chamber separately as it is described in previous chapters, i.e. setting up sources and substrate motion. One can add, delete, duplicate stages and/or change their order.

4. Analysis of the results

The output of Make Process simulations are relative values fluxes of each source to the substrate as a function of substrate position as well as energy and angular distributions of condensing particle for each substrate position. The data can be used in film growth simulations. Also, the time evolution of coating thickness is another output of Make Process simulations. All output data files are stored in YourProject\ plugins\MakeProcess\output folder.

Let us look at a simple example of a coater with two sources and a substrate placed on a rotating table, see Figure 3

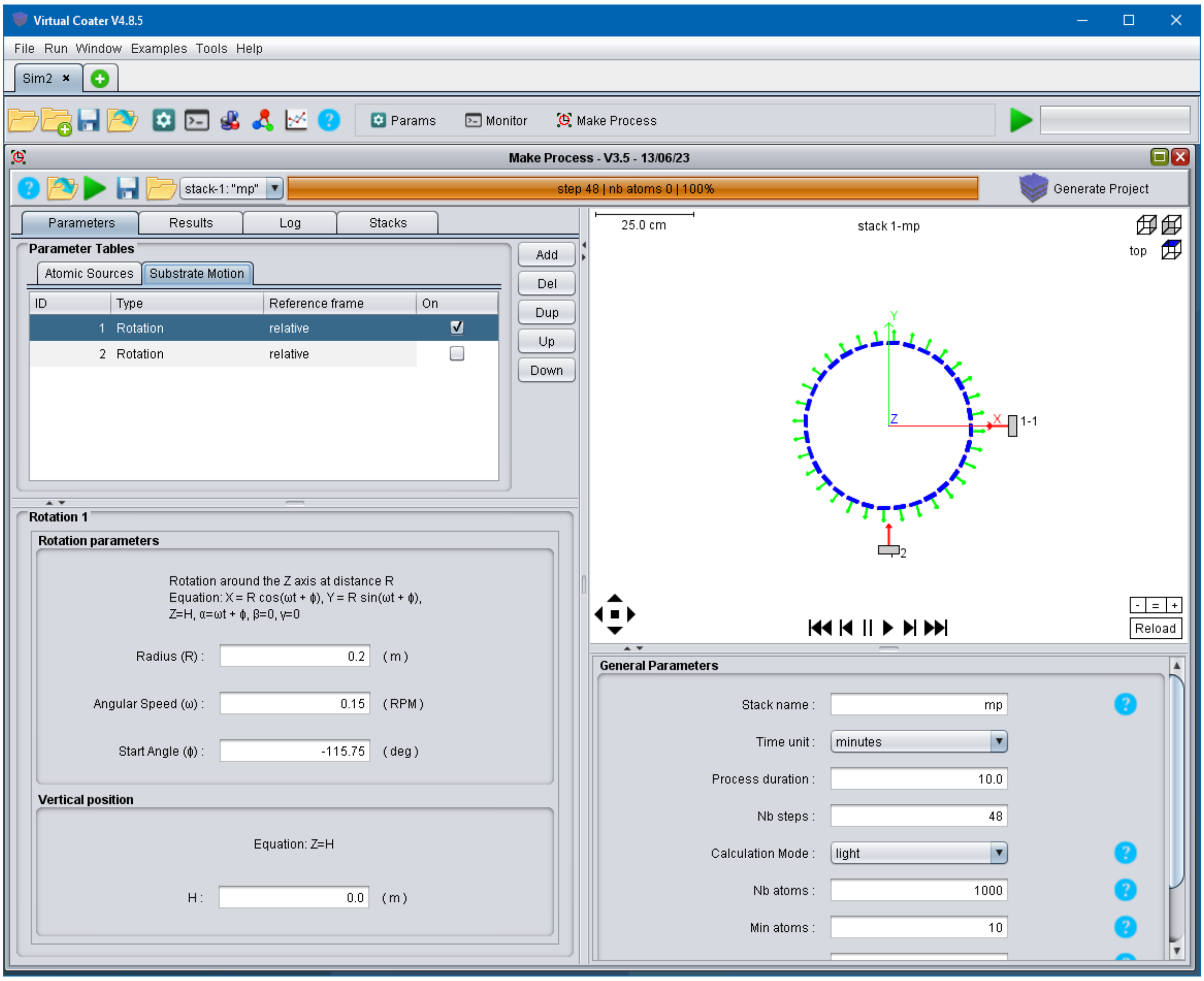

Figure 3 A double magnetron coater with a rotating table.

Examples of the output for the case are presented below, see Figure 4.

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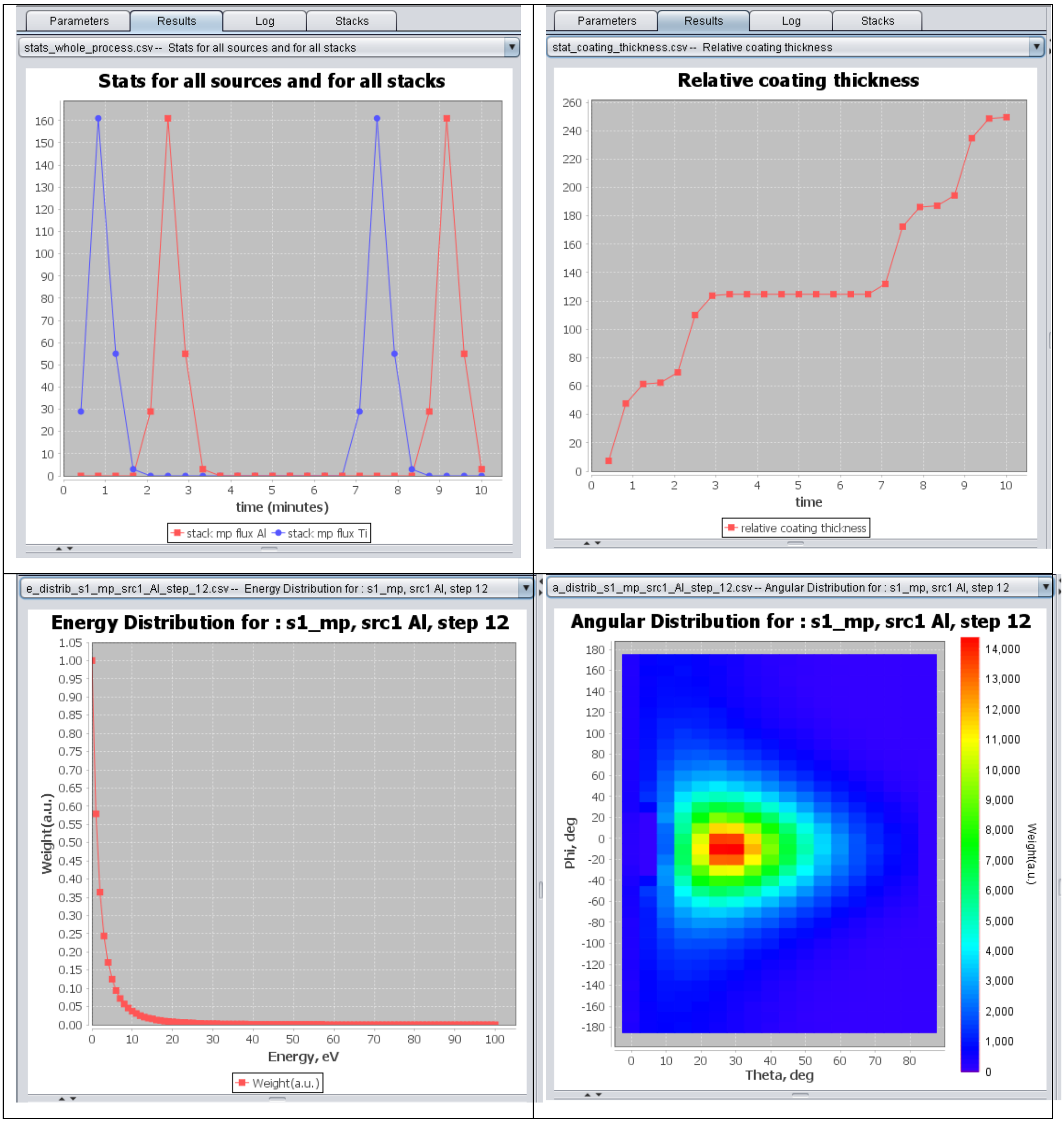

Figure 4 Output of Make Process. Top row, fluxes from Ti and Al sources to the substrate as functions of time (left) and thickness evolution of the coating. Bottom row, energy and energy distribution of particles which are condemышmп at the substrate at a its given position.

4.1. Fluxes

Let us analyze briefly these results. From the Figure 3 one can see that the rotation speed of the table is 0.15 rotation per minutes, starting place is located at -115 degree, i.e. is near Magnetron 2, and the deposition time is equal to 10 minutes. That means the substrate makes

1 and a half rotations passing twice in front of each magnetron. The moment when the substrate is right in front of a magnetron corresponds to a maximum of the flux from the magnetron to the substrate, as we can see in Figure 4 (top left plot). Maximum of fluxes correspond to fast increase of the film thickness, and the time interval with zero flux corresponds to a plateau in coating thickness plot, Figure 4 (top right plot).

4.2. Angular distributions

Angular distribution plot represents angular distribution of condensing particles, Figure 4 (bottom right). For most position atoms come to the substrate at an oblique angle, as one can easily see from geometrical considerations. Thus, there is a “hot spot” in the plot which represents the maximum of the distribution. According to the simulations atoms arrive at the substrate in the given position mostly at about 30^0.

4.3. Energy distributions

Similarly, energy distribution plot represents energy distribution of distribution of condensing particles, Figure 4 (bottom left). Energy distribution depends on pressure as well as target-substrate distance. The distribution is shifted to larger energies in case of higher pressure and/or target-substrate distance, and it is shifted to lower energies otherwise. **Note, that when simulations are performed in light mode, that dependence of the energy distribution on pressure and target-substrate distance is not calculated. Thus, for the precise results always use a full mode.**

5. Make Process and film growth simulations

There are ways of using the output of Make Process for film growth simulations. The first way is used when one wants to simulate film growth at a single position at a moving substrate. In this case one should just click a button “Generate project” at a top right angle of Make Process window, see Figure 1. After that, a multi-layer project will be automatically created, and to run film growth simulations one should only click a “Run” button. All the data regarding relative fluxes, energy and angular distributions for each position of the substrate will be transferred to the project. For the details of setting up film growth simulations with

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Virtual Coater see “NASCAM Manual”. This is the most common and simple way of using the output of Make Process for simulations of film growth.

The second way of using the output of Make Process for simulations of film growth simulations is used when one wants to analyze film properties, such as thickness and/or morphology of coating at different places at a fixed non-moving substrate. In this case every position of a “simulating moving substrate” should be regarded as a separate location at a real fixed substrate. After doing Make Process simulation one can use every set of energy and angular distribution calculated for a given substrate position for performing film growth simulations at this position at the substrate.

Let’s look at an example, see Figure 5 . In the example one wants to analyze film properties at different positions on a non-rotating roll.

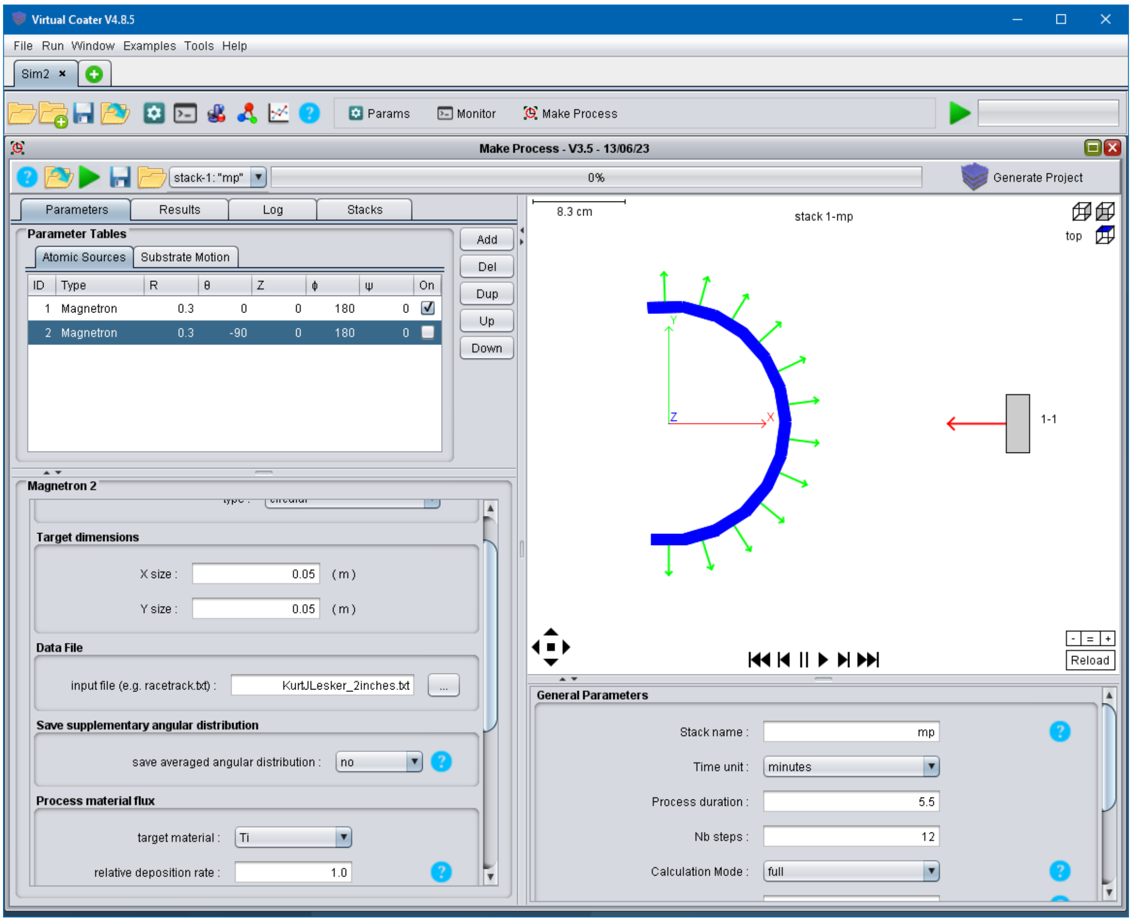

Figure 5 Deposition on a non-moving roll.

First, one can use “Results” tab to see the dependence of a deposition flux on the position on a substrate, see

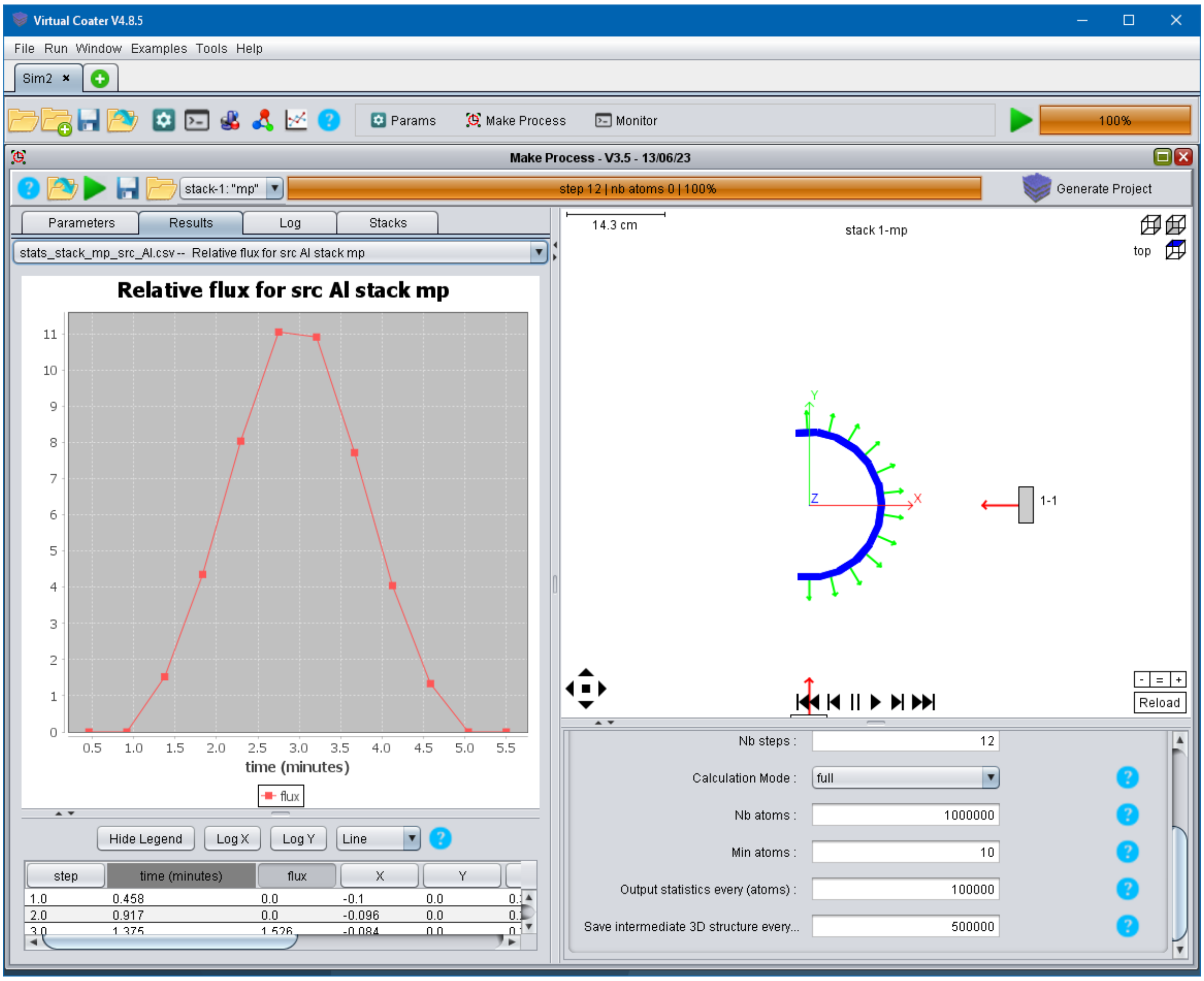

Figure 6.

Certainly, the thickness of the film is proportional to the flux. In addition, thickness of the film depends on the coating density, the higher the density, the lower film thickness,

$$h \sim F/\rho,$$

where h is the film thickness at a given position, F is the flux to the position, and ρ is the coating density at the position. Thus, one can see that to determine the thickness profile across the whole roll one has to run film growth simulation in order to get the dependence of the coating density at each position at the substrate.

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To run film growth simulation for a given position at the substrate one should use angular and energy distributions calculated by Make Process for this position. Certainly, it is necessary to run such simulations for each position, manually setting them up. Fortunately, Virtual Coater enables running these simulations all at once or part by part, depending on the number of cores/processors in a computer.

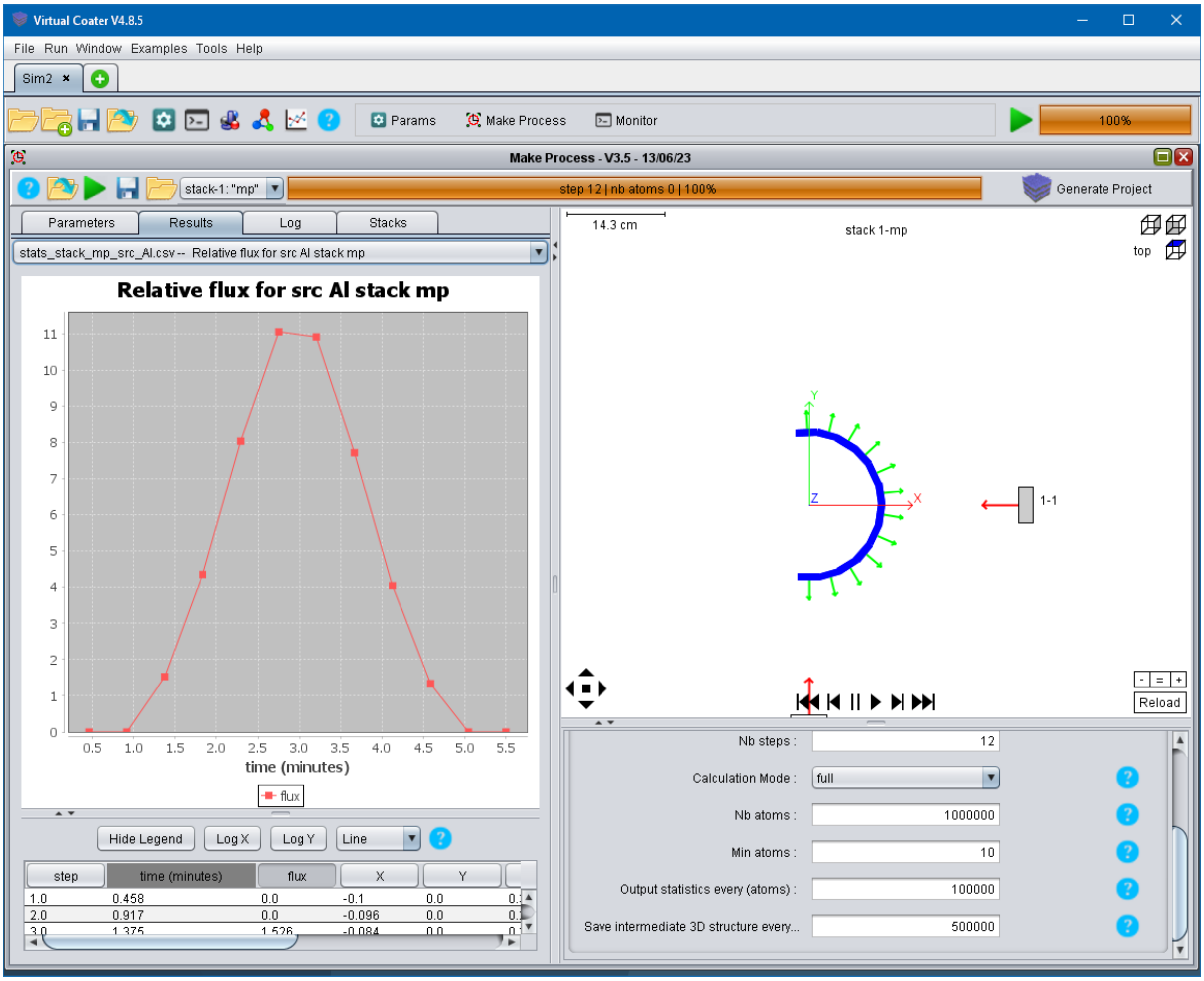

Figure 6 Dependence of a deposition flux on the position on a substrate.