



SYSTEMA OUTGASSING

Version 4.9.0

User Manual

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Introduction

Scope of the document

Some materials - such as glues, paints, and MLI (Multi-layer insulation), react in space vacuum environment and might reject couple of chemical species during the satellite mission due to evaporation reactions (outgassing phenomena).

Systema Outgassing V4 is a module of Systema suite dedicated to the molecular contamination analysis of space systems. The aim of this module is to estimate which type of chemical species are the most contaminant in a satellite/instrument for each sub-systems and to compute levels of contamination to ensure the spacecraft liability to face molecular contamination during the mission lifespan.

The purpose of this document provides a user tutorial in order to handle Outgassing module and to correctly conduct a contamination analysis on Systema V4.8.0. **Molecular contamination theory is not detailed in this document.**

Outgassing analysis description

The contamination analysis method using Systema V4.8.0 is performed through the following steps:

- 1- Geometrical modelling of the spacecraft
- 2- Meshing creation of the geometrical model
- 3- Outgassing properties assumptions
- 4- Material descriptions (from database)
- 5- Multi-material description
- 6- Distinct side description
- 7- Mass Transfer Factor computation
- 8- Mass Deposit calculation
- 9- Bake-out computation
- 10- Post-processing

The following figure summarizes the whole contamination analysis process which has to be conducted to perform a contamination simulation on Systema V4.8.0.

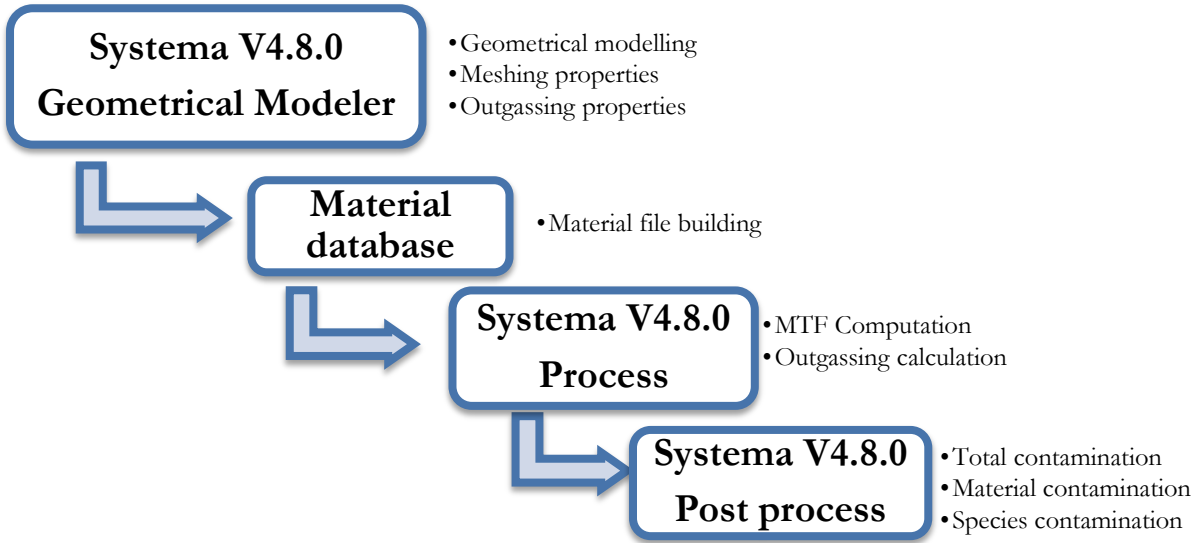


Figure 1: Systema Outgassing V4.8.0 analysis process

All these steps are detailed in dedicated parts of this document.

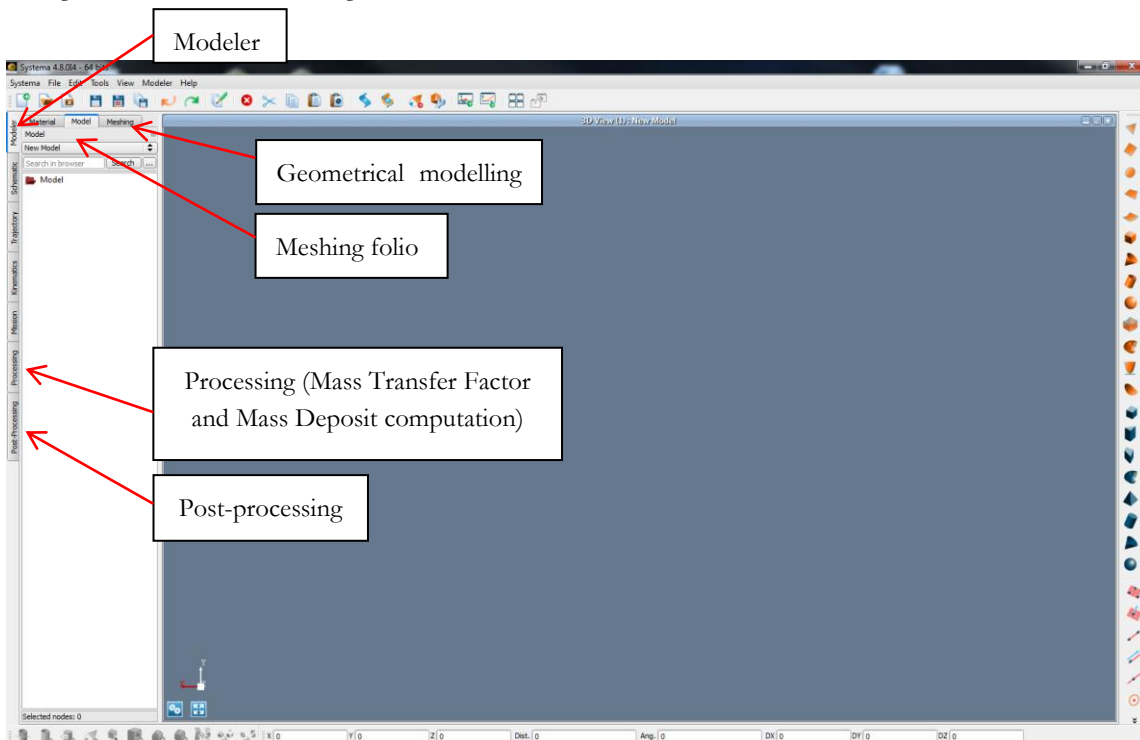


Figure 2: Systema V4.8.0 Interface presentation

1 Geometrical modelling

Outgassing geometrical models can be fully designed on Systema V4.8.0 with the geometrical design module. Nevertheless, geometrical models for outgassing are rarely entirely designed by the user. In most of case, a thermal geometrical model used for Systema Thermica computations is provided, or in some cases geometry can be provided by STEP files.

1.1 Modelling from thermal geometrical model

First, it is recommended to open the provided thermal model (.sysmdl) on Systema Thermica and to remove all coating properties. In that purpose, select the root of the model and click on the “Remove Thermica property in children” in Thermica.



Figure 3: Thermica modelling toolbar

The required geometrical model for an outgassing computation has different requirements from a thermal geometrical model as outgassing results are entirely led by the ray tracing computation. Most important rules to avoid inactive impingement (refer to §0) are listed below:

- Any closed cavity (or box) must be perfectly fitted in the geometrical model; else emitted particles might be loss outside the cavity.
- Shapes are defined by two faces which can be defined as active or inactive. Inactive faces are acting as a non-emitting/reemitting surface, i.e. any ray impacting such a surface will be lost, compromising the global mass conservation.

1.2 Modelling from STEP data

In that case, geometrical model must be built entirely thanks to this model. Only the required geometries must be kept. The main point is to discuss previously with projects managers of the required subsystems to model and level of accuracy. Every geometrical simplification must be of course validated. Mounting pieces such as bolts, screws etc. are not necessities. It can be kind to close tiny holes and to ignore tiny equipment, particularly if those are metallic. Keep in mind that outgassing computations are very long (sometimes up to couple of weeks) and every geometrical simplification is welcome as long as the global geometry is representative.

In both cases:

Globally, beware of every adjacent surface, particularly those defining closed surfaces if their internal faces are inactive. Quadrangles and triangles shapes are much recommended to ensure the surfaces enclosure.

Cutters (to cut holes in shapes) are very convenient to model venting holes or complex geometries. But beware that holes open closed surfaces, consequently internal faces of an opened volume must be active in that case.

It is recommended to group every sensitive item (studied devices in the purpose of the outgassing analysis) in a same object to make the post-process of results easier with labels (Refer to §2 and §9.1).

By the way, to make a cleaner model and to make it more readable, it is preferable to create as many object as possible to detail the model tree especially if those includes several shapes. A random example of model tree organization is given on the right.

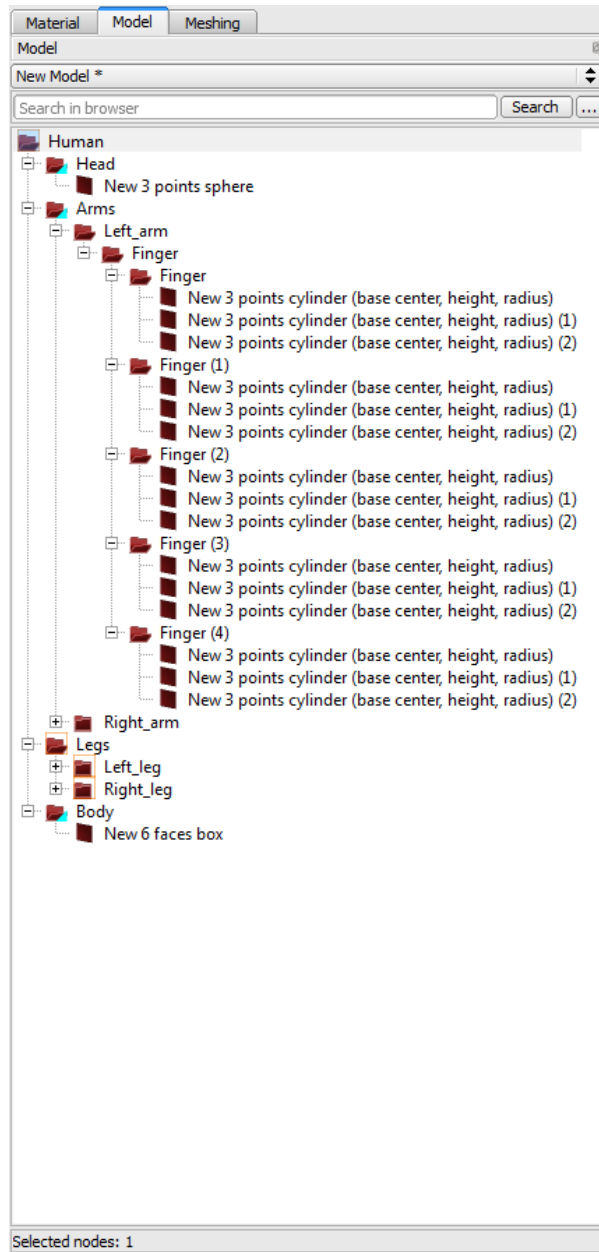


Figure 4: Example of model tree with several objects defined

2 Meshing construction

Every shape is automatically meshed by the software. Beware that the mesh auto-numbering might be changed if new shapes are created/deleted or if the geometry is re-organized. It might impact post-process result extraction furtherly, especially the group definition (Refer to §9.1).

A shape is defined by two nodes by default corresponding to front and back faces, but nodes corresponding to inactive faces are not declared for the Mass Transfer Factor computation and will not appear in .dck file (Refer to 7-).

The meshing must be finer in sensitive areas such as small cavities or venting holes. Moreover a fine mesh can be useful to study the particle propagation (in a pipe or around a venting hole for example).

As the mass deposit is being modelled as a density, the reemission of particles can happen anywhere on a nod. Consequently, the user should make the meshing more detailed if necessary, particularly to avoid molecular leaks in some cases as example in the following figures:

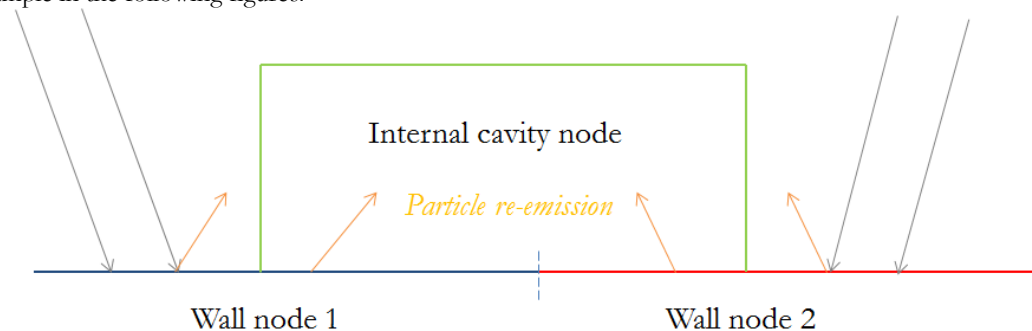


Figure 5: Example of particle leak inside an internal inactive box

If the internal face of the cavity node is inactive, the particle leak inside the cavity brought by node 1 and node 2 will induce particle disappearance. Cut and/or finer mesh is required in that case.

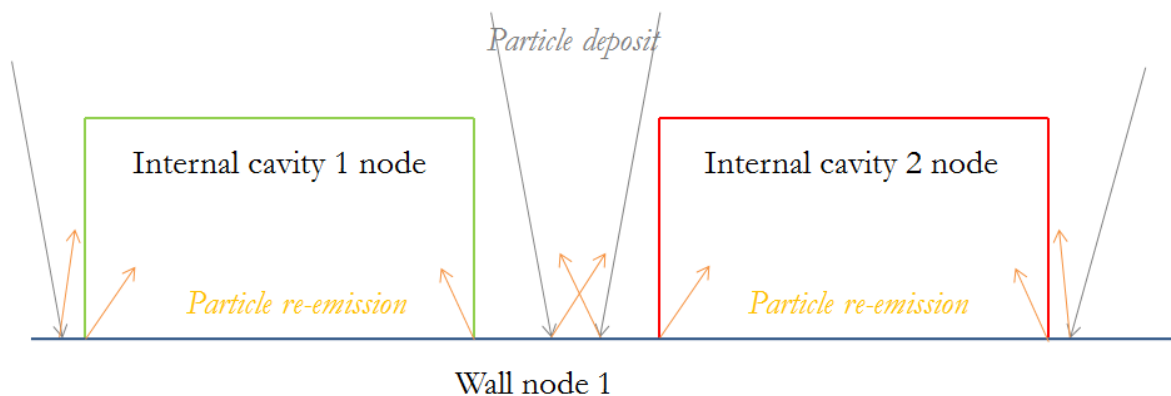


Figure 6: Example of particle leak between two independant boxes

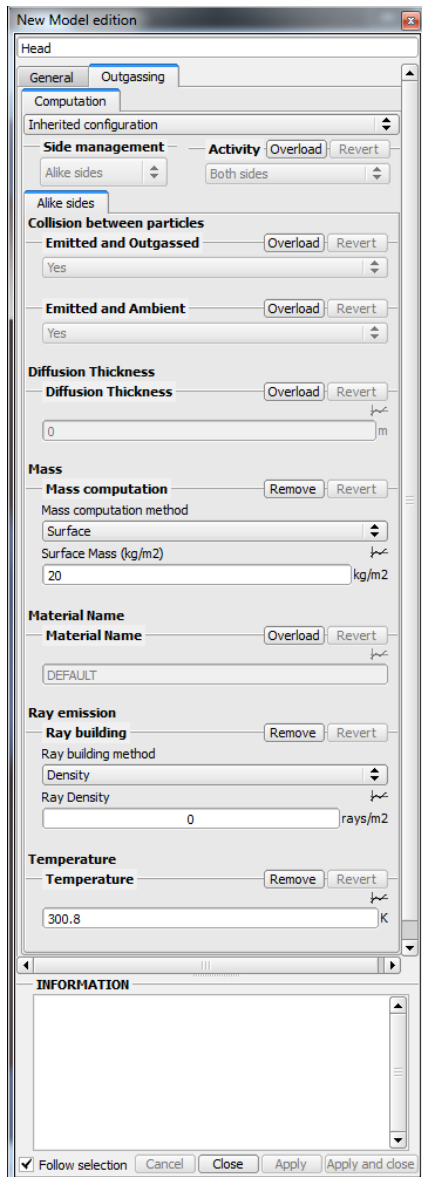
If the same node is defined in the bottom of two independent boxes, it will make a link of particle reemission between both boxes which are not isolated anymore. In that case, there must not be common nodes between both cavities.

Finally, a “Label” can be assessed to group several nodes to study the contamination on the whole group. Overload and modify the “Label” definition in the meshing properties of a shape (or better, of an object). **Beware of not defining label as a substring of another one (for example “Leg” is contained in labels “Leg_1”, “Leg_2”... (refer to §9.1))**

3 Outgassing assumption properties

By double-clicking on a shape (in the “Model” folio), “Outgassing” properties are displayed and can be modified by the user. By choosing “Inherited configuration”, common properties can be assessed to a whole group of object by editing its own properties.

Mandatory outgassing properties to be defined are the following ones:



- “Mass computation”: Assigned in areal mass (kg/m^2) or bulk mass (kg). Beware that if both sides of a shape are active, the shape area is considered for both sides. For instance, $10\text{kg}/\text{m}^2$ on a 1m^2 shape (with both side active) involves 10kg on side 1 and 10kg on side 2: total 20kg. The bulk mass of a shape is assigned to one face if only one face is active and it is divided equally among the two faces if both faces are active. Note that if a box with a bulk mass of 1kg is created, it is equivalent to a cube of which each side has 1kg instead to a $1/6\text{kg}$ per side.
- “Material name”: Assigns a material name. One different material name can be used for different device in case of cross-contamination (even if it’s actually the same material) in order to distinguish the provenance of outgassed species in case of cross-contamination. The name of each material must be consistent with the `material.dat` file (refer to §4-). It is preferable to avoid long names for materials (below 24 characters). DEFAULT material is used by default. Mass must be kept at 0 kg if no outgassing computation is needed.
- “Ray emission”: Number of ray fired per mesh to compute MTF. An interesting way is to define a low amount of ray (10^3) to check the model before using a huge amount of ray (10^6) for the computation.
- “Temperature”: Temperature of the surface (defined in K). Transient temperatures cannot be easily modelled yet (refer to MTF computation 7- for more details).

Do not forget to “Apply” after changes else modifications will be lost!

Figure 7: Outgassing properties of shape definition

A warning will appear on the shape description if these mandatory inputs are not consistent. However, if the mass computation is kept at 0 kg, the following warning appears “Warning: A mandatory property is not valued: Outgassing>SHELL>Computation>Alike sides>Mass>Mass computation”. In case of the material is “DEFAULT”, this warning is not relevant

4 Material definition

Every material defined in the geometrical model (refer to §1-) must be found and defined in a `material.dat` file which will be called for the outgassing computation.

The material file contains outgassing properties of each species. The properties defined are not identical depending on the type of definition of the material so beware of the source of material data (ESA or CNES database).

A couple of example of material definition is given in the figures hereafter (physical annotation are not detailed, refer to the outgassing theory):

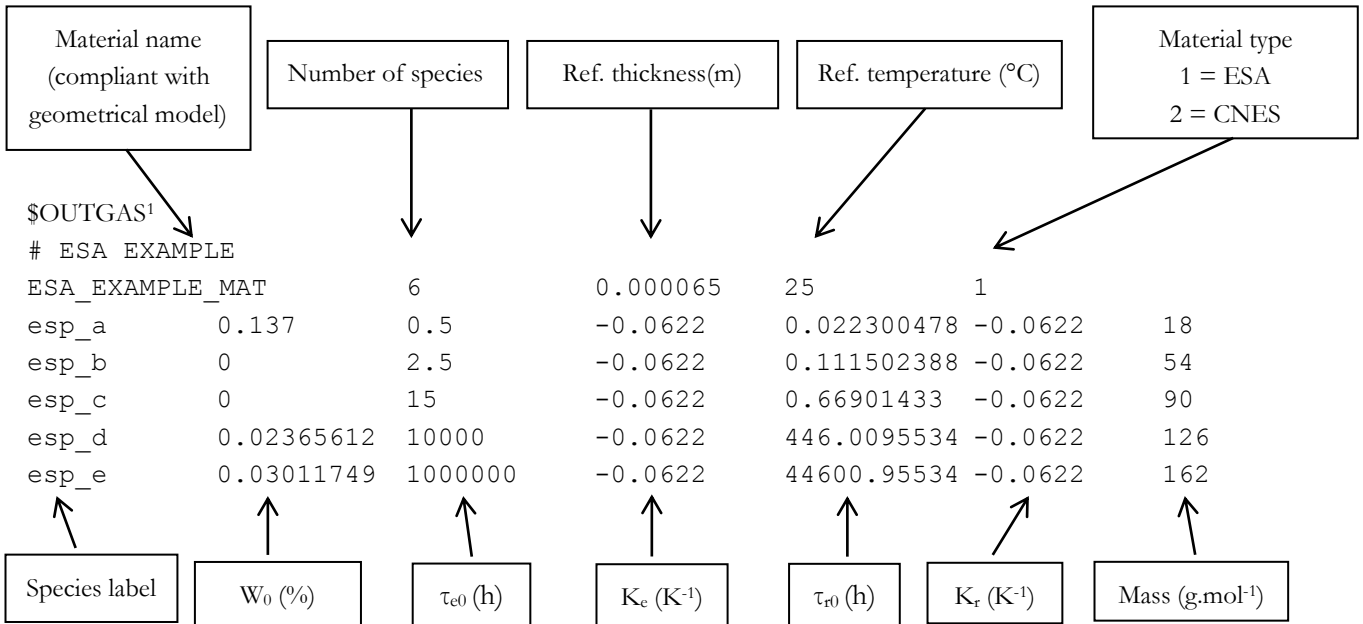


Figure 8: ESA Material definition

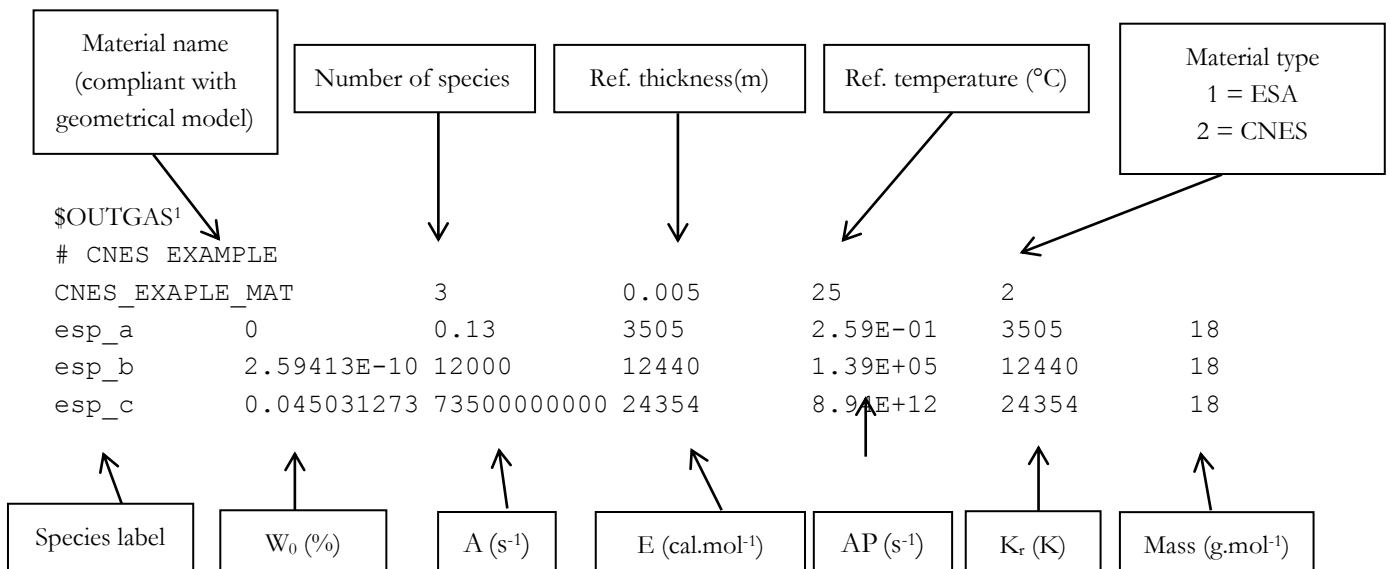


Figure 9: CNES Material definition

¹ Mandatory on the first line in the `material.dat` file to allow the outgassing calculation.

Multi-material definition:

In specific case, a material name defined in the geometrical model (refer to §1) can be defined by two different materials. The user could use the following instructions to take into account the multi-material properties. In the `material.dat` file, the user had to add some information. An example of multi-materials definition is given in the figures hereafter:

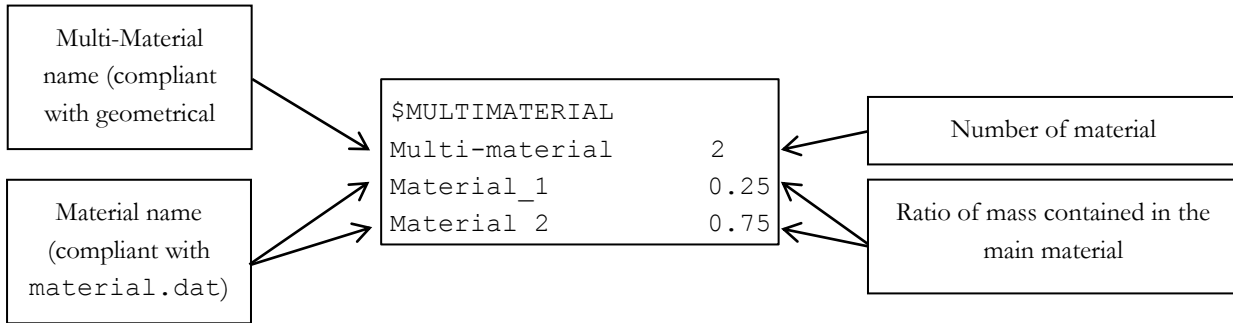


Figure 10: Multi-material definition

5 Distinct Side definition

By double-clicking on a shape (in the “Model” folio), “Outgassing” properties are displayed and can be modified by the user. By choosing “Local configuration”, and then choosing “Distinct side” in “Side management”, two different materials can be applied on each side (positive and negative sides) of the same shape.

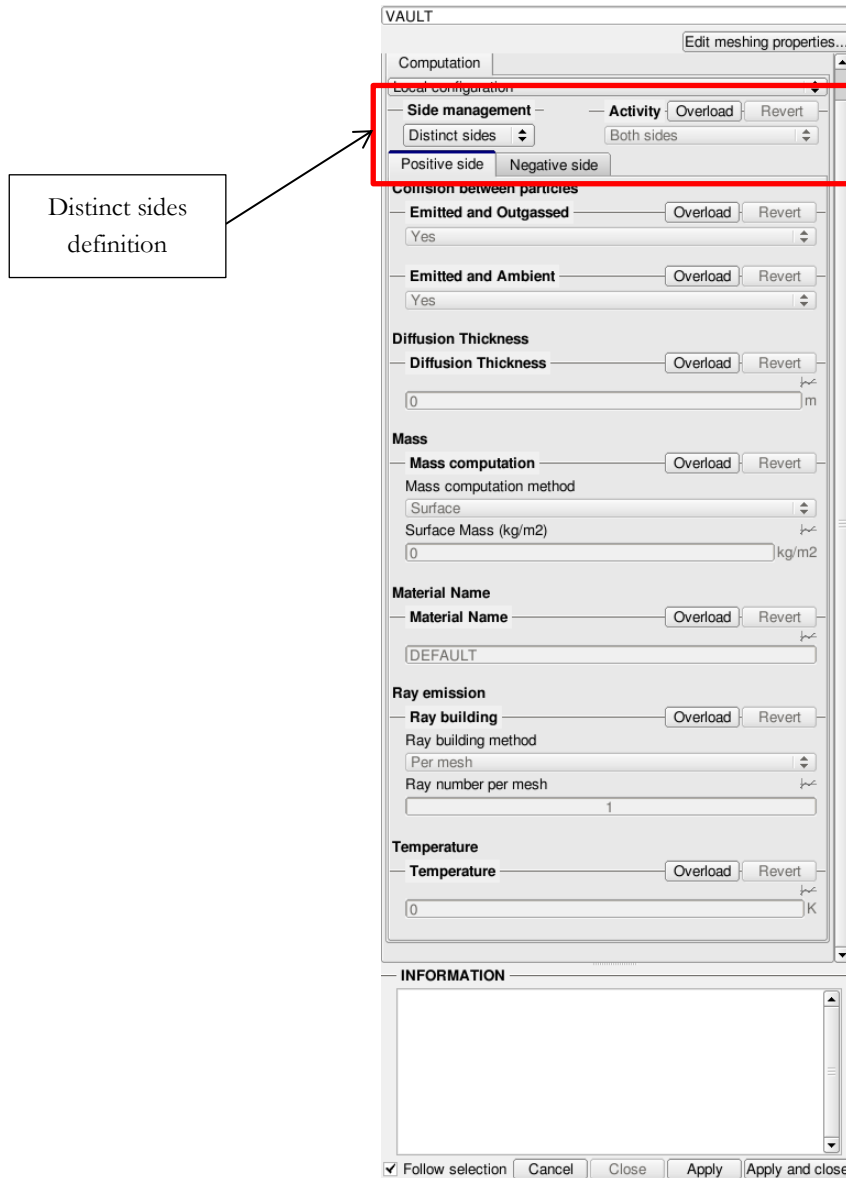


Figure 11: Distinct side definition

Do not forget to “Apply” after changes else modifications will be lost!

6 Mass Transfer Factor Computation

Mass transfer factor computation box is available in the “Process” part of Systema V4.8.0 (refer to Figure 2).

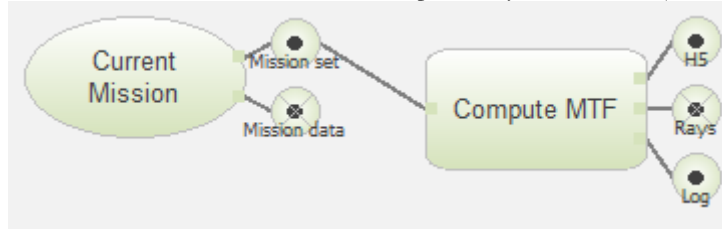


Figure 12: Mass Transfer Factor computation process diagram

The “Current mission” box requires a type of exported structure in which a meshing file (.sysmsh) corresponding to the case of study must be declared.

The “Compute MTF” box requires all ray-tracing parameters displayed on the figure below in order to compute mass transfer factors.

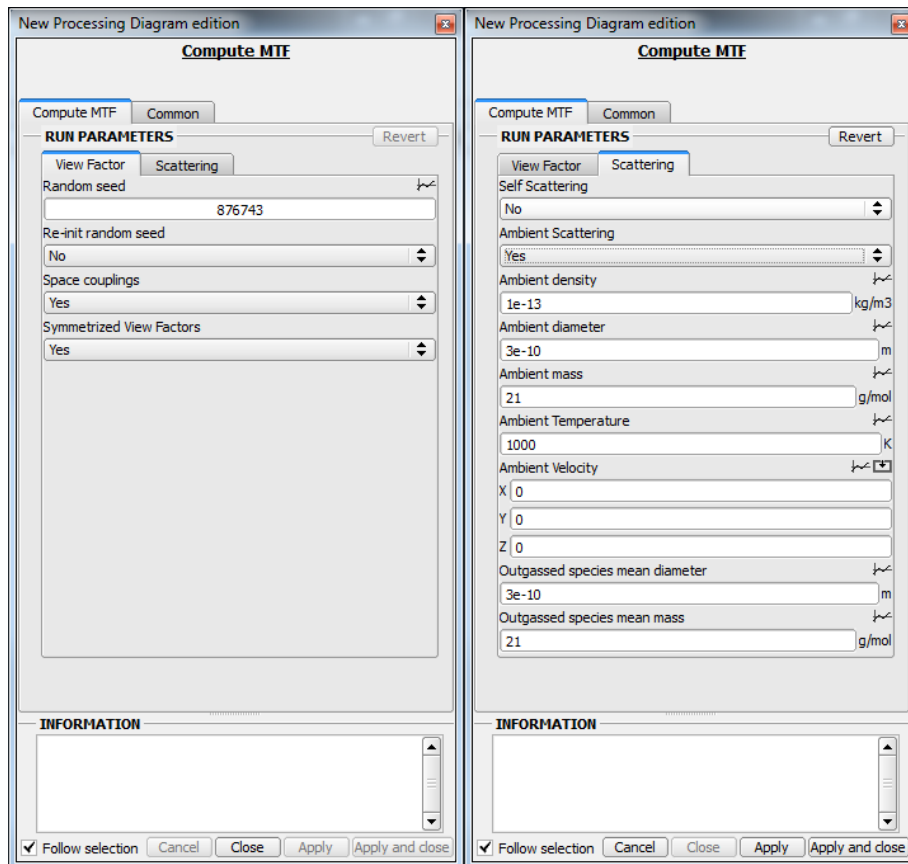


Figure 13: “Compute MTF” parameters

Remarks:

- In most of case it is preferable to NOT enable the View factor symmetrisation to ensure the mass conservation.
- Self-Scattering is not available yet.
- Ambient Scattering is available and requires several data about environment contaminants which can be determined with “Environment” module of Systema V3.2.

The “Generate DCK” box takes as input the “Compute MTF”’s h5 output and the `material.dat` file defined manually (refer to §4-).

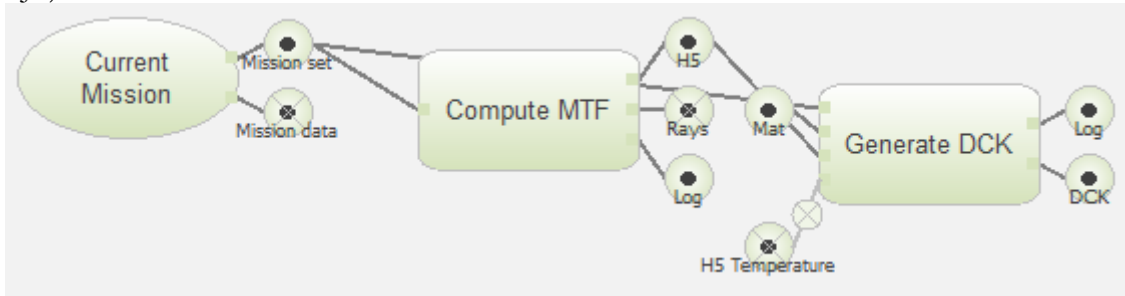


Figure 14: DCK Generation process diagram

This step computes the required parameters concerning time-step calculations and outputs.

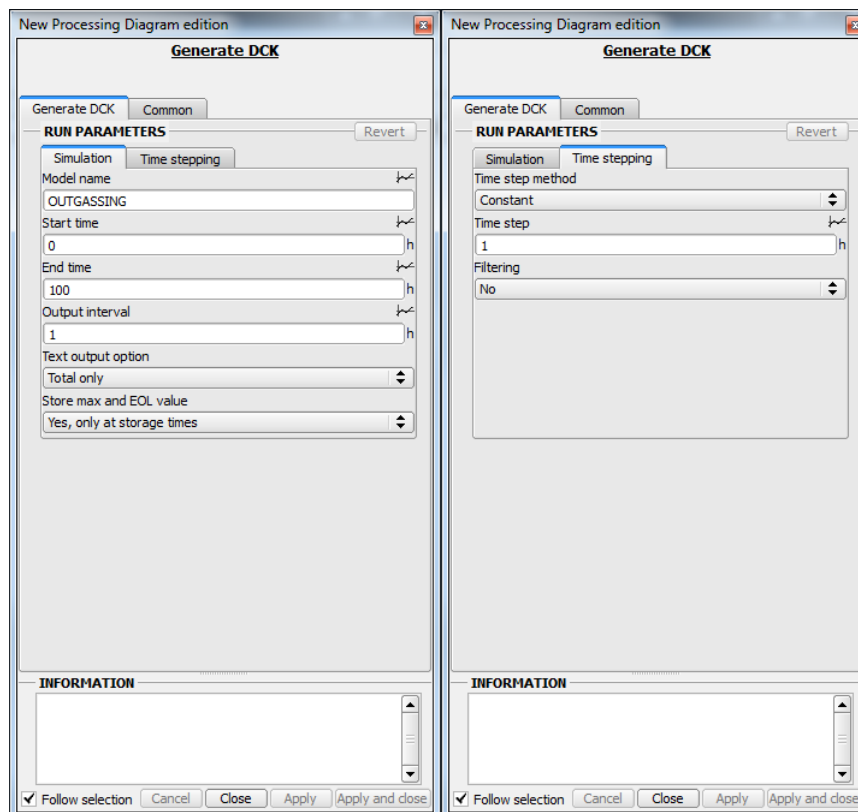


Figure 15: "Generate DCK" parameters

Do not forget to confirm all your choices by clicking on “Apply” button; else changes will not be stored.

Remarks:

- Check `.log` file generated by the `.dck` computation. The inactive impingement budget must be as low as possible. It represents inactive impacts that occur during the MTF computation. A high amount of inactive impingement (>30%) is unconceivable to perform an Outgassing simulation. In most of case it represents a loss of mass due to inactive surfaces (which can be detailed in the log file). Check again accurately the surface enclosures in the geometrical model. Use a low amount of fired ray to perform this model correction step and make a final check with an actual ray number (10^6).

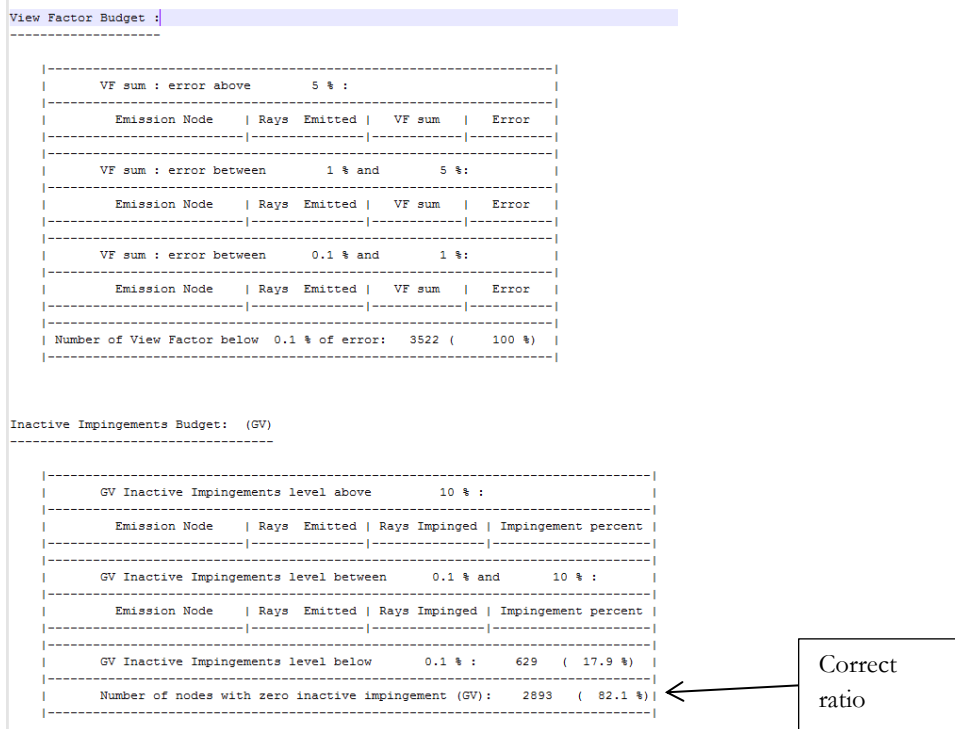


Figure 16: Log file for an acceptable MTF computation

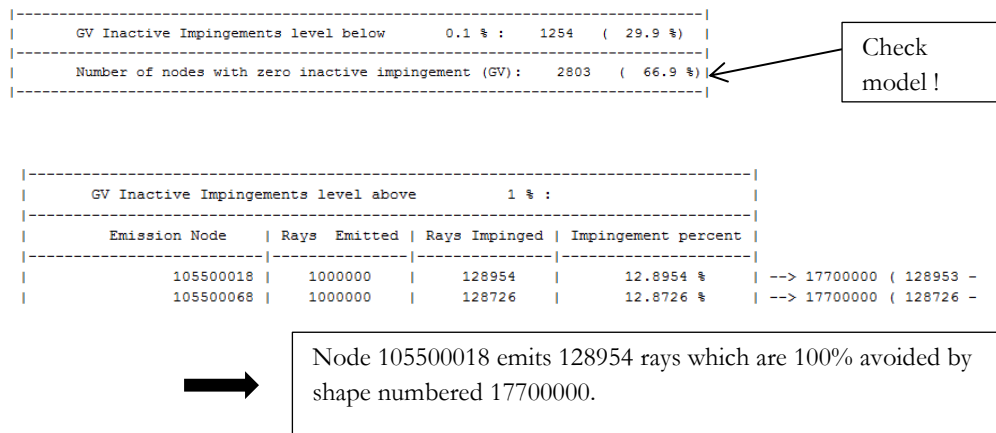


Figure 17: Log file for a high inactive impingement MTF computation

- End time, Output interval and Time step are usual simulation parameters. Output interval must be larger than time-step. More, it's highly recommended to choose a multiple of time-step as output interval.
- The .dck file generated through this step contains all species definition, node declaration (without inactive nodes), view factor computed values, and some outgassing parameters (mass computations, time inputs, outputs).


```

**TYPE** cycles
**TIME STEPS**
0. 24. 48.0 72.
**END TIME STEPS**
**RULES**
/cryostat/vessel/external          280 250 245 200
/cryostat/vessel/viton             300 250 250 200
/cryostat/vessel/window            320 250 230 200
/cryostat/vessel/struts_baffle     300 250 230 200
**END RULES**
**INPUT**
DCK_FILE_RELATIVE_PATH    ./microcarb.dck
**END INPUT**
**OUTPUT**
FORT93_FILE_RELATIVE_PATH ./fort.93
**END OUTPUT**
  
```

Figure 20: Example of input for generate_fort93.py script

The structure of the previous file is the following:

- Let the section ****TYPE**** unchanged
- The section ****TIME STEPS**** must contains a list of float number that represent the time of the simulation when the temperature is changed.
- The section ****RULES**** contains
 - o The path in the Systema model to the considered object
 - o The list of temperature to apply to this object during the simulation. The temperatures must correspond to the time list of ****TIME STEPS**** section
- The section ****INPUT**** contains as an input the path to the DCK file generated in the first step.
- The section ****OUTPUT**** contains as an output the relative path to the fort.93 file.

To execute the next step, the users should launch, with the meshing open, in Systema V4.8.0 the following python script:



Figure 21: Python file for fort.93 file creation

In that purpose, select the button “Launch python script” and open the “extract_nodes_for_fort93_class.py” file.



Figure 22: Systema V4.8.0 toolbar

Before to launch the script, the user had to:

- Open Systema V4.8.0;
- Open the meshing.
- Have generated a DCK file with the H5 temperature option deactivated.

Once the file is created, it is mandatory to rename it: “fort.93”.

The mass deposit computation could now be launch. For further information and operating instructions, please refer to the §6.

The user must finally load the fort.93 file in the “H5 Temperature” cursor. In that purpose, the user must right-click on the H5 temperature and select “Activate file”:

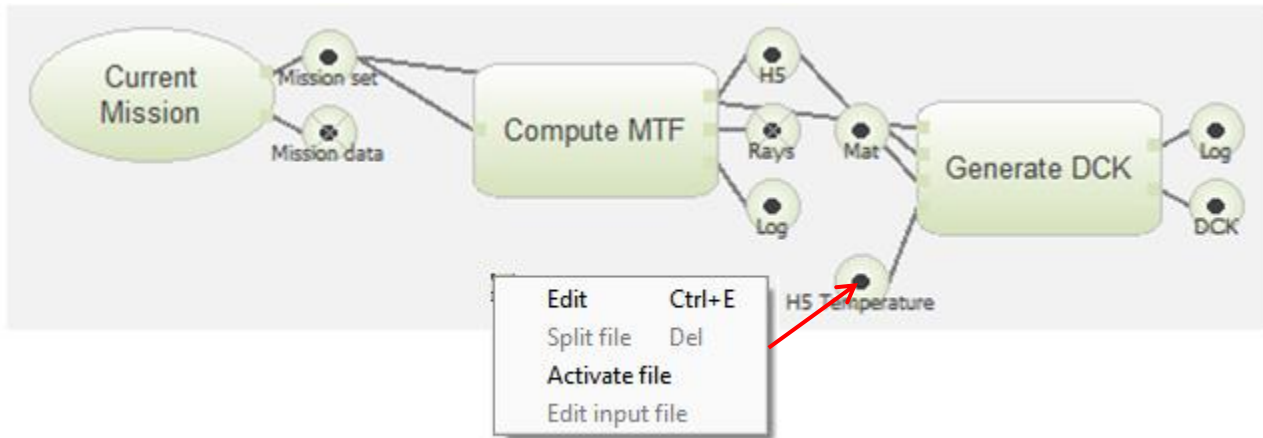


Figure 23: fort.93 file analysis diagram

The user could now select the fort.93 file in the “H5 Temperature” parameters. Do not forget to confirm by clicking on “Apply” button; else changes will not be stored.

7 Mass Deposit computation

An outgassing computation can be performed using the “Mass Deposit” as soon as the .dck file has been generated correctly and the model could be validated with an allowable inactive impingement ratio.

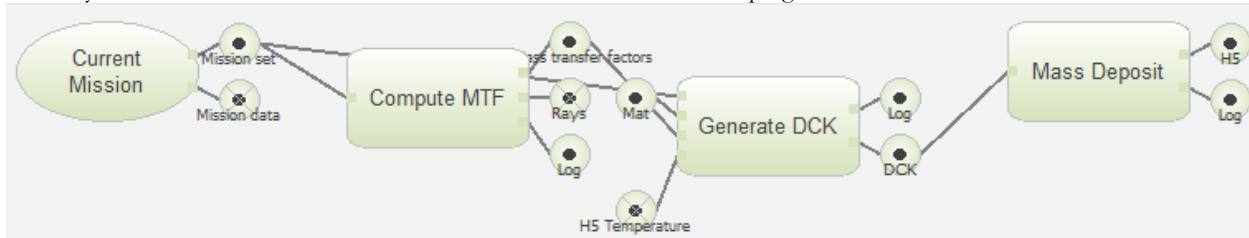


Figure 24: Entire Outgassing analysis diagram

The “Mass Deposit” parameters are listed below:

- Solver/“Global case list”: Defines the species which must be computed for the analysis. The number of each species is defined in the .dck file.
 - o “ALL” by default performs a computation for all species.
 - o Ranges such as 3-8 will compute mass deposit of species 3,4,5,6,7,8.
 - o 1,2,6-10,12 will compute mass deposit of species 1,2,6,7,8,9,10,12.
- Solver/“Computation Scheduling”:
 - o Parallel: Multi-CPU computation (1 specie/CPU) – allocated number of CPU can be changed by changing the value of Systema environment variable SYSTEMA_NTHREAD.
 - o Sequential: Single CPU computation (not recommended).
- Results/”Store mass density”: Choose the unit of result computation.

Do not forget to confirm all your choices by clicking on “Apply” button; else changes will not be stored.

A .csv file, a .log (computation process) file, .out file, and .h5 (data storage) file are generated during the computation of each species.

Computation time may be very long. It can be useful to have a look at those files to follow the calculation progress:

- The .out file allows the user to check the consistency of the computation during each time step (emitted mass and percentage of error on mass conservation). An inconsistency in this file can reveal the existence of an error in the model.
- The .csv displays the calculation progress to the user. A very huge number of iteration (100+) at each time step reveals some difficulties to reach the convergence criteria of the solver.

At the end of the computation, “Mass Deposit” will compile a global .h5 file containing all concatenated .h5 stored in the result directory (huge file, up to 10Go).

8 Bake-out computation

A bake-out computation can be performed using the “Bake-out” box in the processing part of Systema V4.8.0. A bake-out is applied at a material and is defined by two parameters, the time of bake-out and the temperature of bake-out.

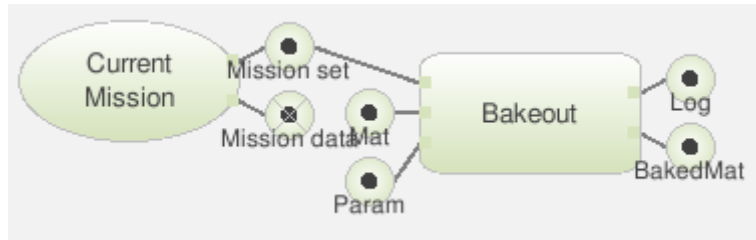


Figure 25: Bake-out analysis diagram

The “Bake-out” input data are listed below:

- material.dat file (defined in §4);
- Another text file named “Param” (see Figure 23).

An example of a list of two material bake-out definition (“Param” file) is given in the figures hereafter:

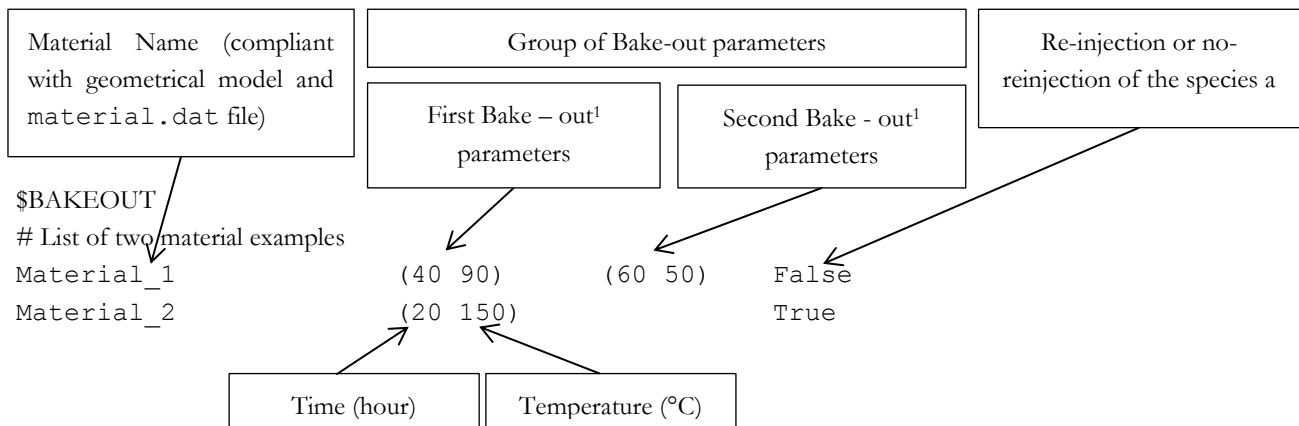


Figure 26: Bake-out description

The output file is a material.dat file, as defined in §4, which could be directly use by the user for the Mass Transfer Factor Computation (§6).

¹ Mandatory on the first line in the material.dat file to allow the running..

9 Post-processing

The post-processing (following steps) can be performed independently from the previous computation as a new diagram must be defined in the post-processing folio of Systema V4.8.0.

The “Sensitive items mean deposit” takes the global concatenated .h5 file as input extracts the contamination data required to study the contaminations of each material or species. Nevertheless, the .h5 file must be added and linked to “Entity” box manually by clicking on “Insert HDF5 file” (See next figure).

Do not forget to confirm all your choices by clicking on “Apply” button; else changes will not be stored.

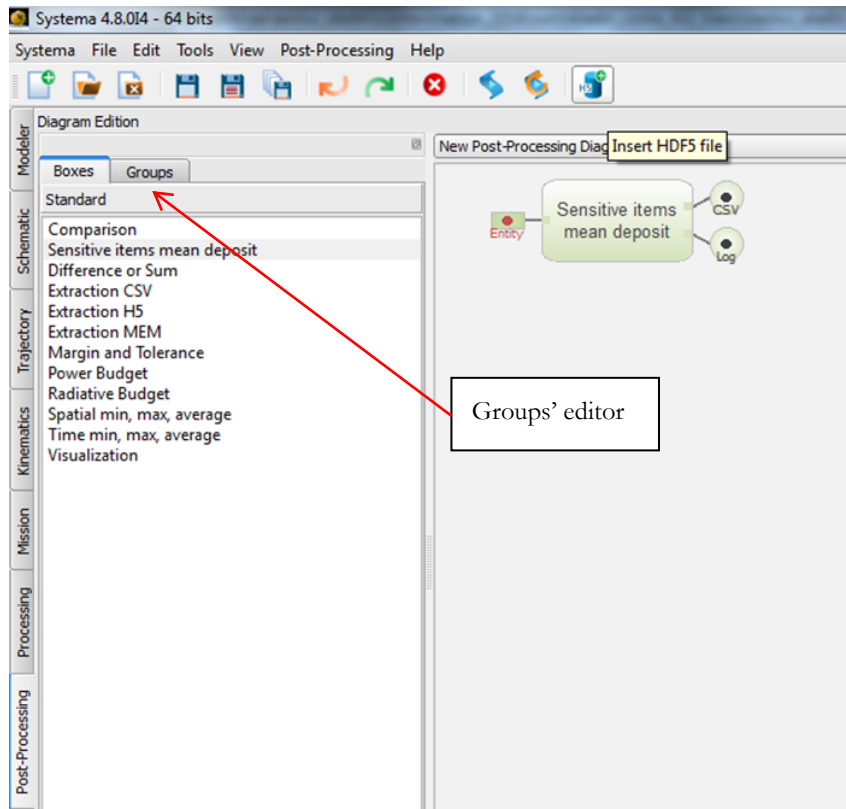


Figure 27: Post-processing interface - Sensitive items mean deposit

9.1 “Groups” definition

Before executing a post-process, extraction groups must be defined (either in a text .txt file or directly in the Groups folio editor – refer to the previous figure). An example of group file to be extracted is given in the figure hereafter:

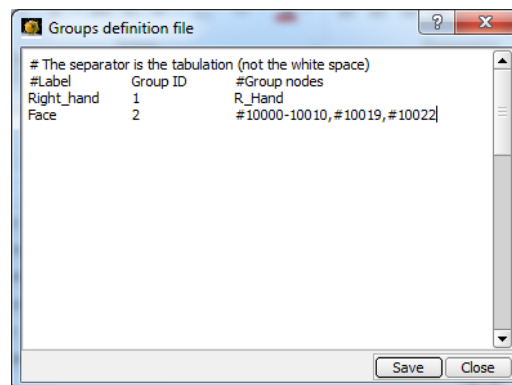


Figure 28: Example of group definition file

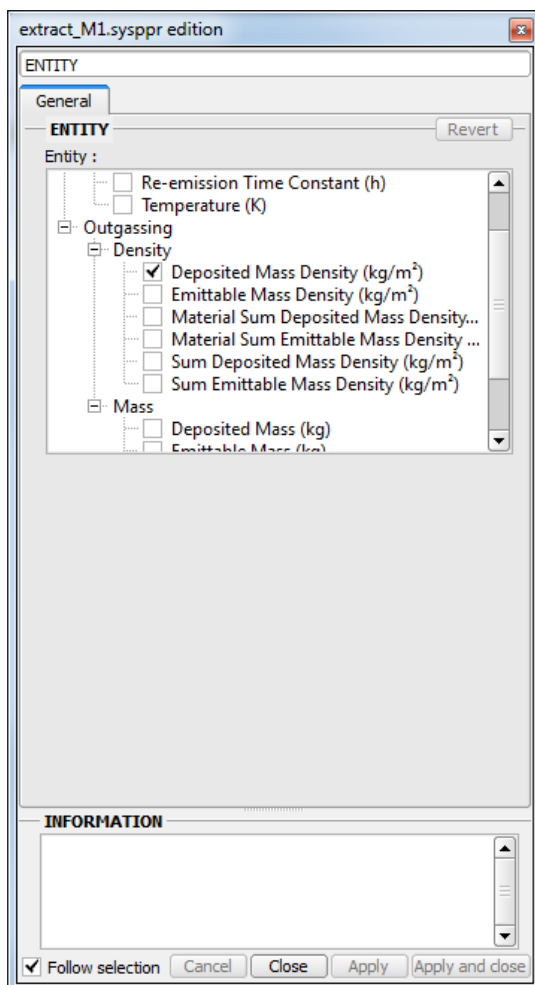
- “Label” is the group name which will appear as header for results extractions, chosen by the user.
- “Group ID” is defined as a number of the defined group, chosen by the user.
- “Group nodes” describes nodes results to be extracted, chosen by the user. Indeed, there are two ways to define group node:
 - o By calling the Label defined previously in the meshing (Ex: “R_Hand”)
 - o By nodes or node ranges, which must be preceded by # and separated by commas (Ex: #10000-10010,#10019,#10022)

Remind that Labels must be different each other in order to avoid results sums. For instance, if 3 entities (objects or nodes) are labeled respectively “Leg”, “Leg_1” and “Leg_2”, post-processing data from group nodes “Leg” will extract and sum results of all these 3 groups as “Leg” is also contained in “Leg_1” and “Leg_2”.

9.2 “Entity” box configuration

The “Entity box” defines the type of data which can be extracted from the .h5 file. **Only one case can be ticked.** Input data can be extracted, such as group’s Area, Emission time constant, Re-emission time constant, or Temperature.

The following outputs can be extracted either in bulk mass (kg) or in mass density (kg/m²):



- Deposited mass (kg)/ mass density (kg/m²):
Species deposit detail along the time
- Emittable mass (kg)/ mass density (kg/m²):
Species emission detail along the time
- Total deposited mass (kg)/ Material sum deposited mass density (kg/m²): Material deposit detail along the time
- Total emittable mass (kg)/ Material sum emittable mass density (kg/m²): Material emission detail along the time
- Sum deposited mass density (kg/m²): Sum of material deposit along the time
- Sum emittable mass density (kg/m²): Sum of material emission along the time
- Total mass (kg): Total mass of contaminant along the time (deposited – emitted)

Figure 29: Entity box configuration

Remark: If more than one type of data is required, another “Sensitive item mean deposit” box can be defined in the same process.

9.3 “Sensitive items mass deposit” box configuration

This box is complementary to the Entity box. Details about output extraction are given hereafter:

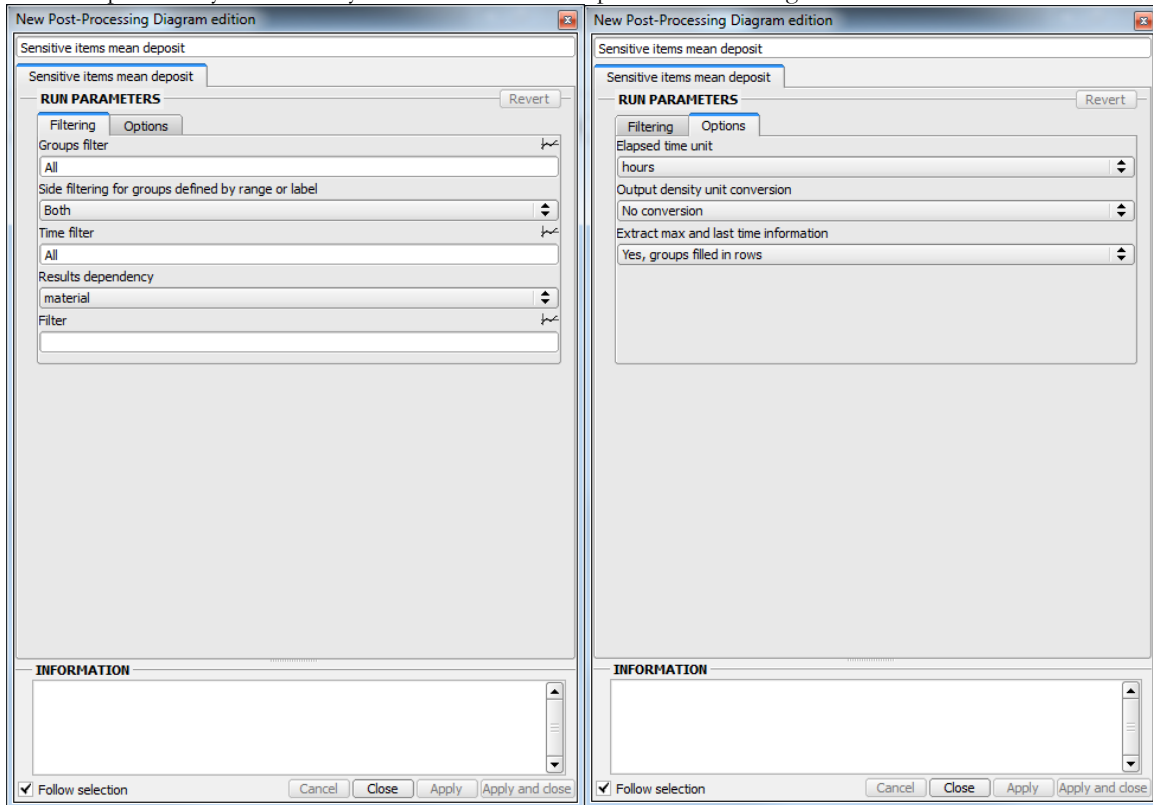


Figure 30: "Sensitive item mean deposit" box definition

- “Side filtering for groups defined by range or label”: Extract results from positive, negative or both sides of all nodes in the group. Beware that all nodes of groups defined in the group file have a similar orientation. If “Both” sides are chosen, extracted data will be summed. If both sides results are needed independantly, two “Sensitive items mean deposit” boxes have to be defined.
- “Results dependency” must be chosen as “material” for extraction of material data or “species” for extraction of species data.

A summary of extracted properties and results dependencies is provided in the following table:

	Entity	Result dependency	Node number available
Properties	Area	None	All (except 997-998-999)
	Emission time constant	Species	All (except 997-998-1000)
	Re-emission time constant	Species	All (except 997-998-1001)
	Temperature	None	All (except 997-998-999)
Outgassing / Mass Density	Deposited Mass Density	Species	All
	Emittable Mass Density	Species	All
	Material Sum Deposited Density	Material	All
	Material Sum Emittable Mass Density	Material	All
	Seum Deposited Density	None	All
	Sum Emittable Mass Density	None	All
Outgassing / Mass	Deposited Mass	Species	All
	Emittable Mass	Species	All
	Total Deposited Mass	Species	997
	Total Emittable Mass	Species	997
	Total Mass	Species	997

Table 9-1: Outgassing properties and results dependencies

Use filters to sift any data concerning a particular group or time range and find data formatting (table orientation, unit conversions...) in "Option" parameters.

Outputs are stored in the .csv file that can be renamed conveniently as well as the log file if several post-process / boxes are defined. Maximum/end time values and contamination plots can be studied from the .csv result file.