OUTGASSING MODELLING: CHALLENGES AND PERSPECTIVES

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ABSTRACT

As widely known in the contamination community, outgassing phenomena is a quite complex process that needs to be modelled and understood in order to quantify its impact on spacecraft.

During a spacecraft design, one can rely on numerical tools that model outgassing physics by taking into account the diffusion of the molecules within the materials, the reflection of the contaminants on the satellite surfaces, the residence time of outgassed species and the sticking coefficient.

OHB, with the support of ONERA, performed a comparison between two numerical tools (used in Europe) that are based on different modelling techniques. This paper will present the validation and its challenges: as example, the residence time of the species can be modelled either with an Arrhenius law or Linearized Exponential.

The article will point out the challenges for modelling the outgassing: the numerical approach greatly depends on the quality of the input that are provided from dynamic outgassing experiments. Plus, due to lack of in-orbit data, EOL data from the simulation are based on “mathematical” extrapolation of species residence time inside the bulk material.

The outcome of the work is that for simple cases, phenomena like importance of reflection versus reemission can be modelled and the results correlated. Once the geometry of the case became more complex, the tools are numerically consistent when compared with each others. However, the two approaches shows discrepancies when it comes to model the volatiles.

The challenges of the contamination due to outgassing is mainly related to the physical modelling. The European approach in this case is to model the spacecraft and minimize the design cost by performing a full-scale analysis. However, lessons learnt showed the limits of this approach: the key point of validation with regard to in-orbit tests is missing.

Perspectives will be that more in-orbit experiments are needed to correlate the simulation and most importantly, cross-match the impact of other processes on outgassing such as Atomic Oxygen, UV radiation and Thruster Plume.

INTRODUCTION

During the last European contamination modelling workshop held in Bremen in February 2017, a roadmap for enhancing the knowledge in this field have been established.

This roadmap is divided in several sections:

- Outgassing modelling
- Numerical modelling
- Experiments techniques (discarded in this article)
- Validation
- Processes (discarded in this article)

Full understanding of the fundamental physics behind outgassing phenomena is a key element. In fact, some key understanding elements are unclear or lacking a solid basis. For example, it is very difficult in practice to identify the prominent process between reemission and reflection. This part is closely linked to the numerical modelling part.

Since years, two numerical tools are widely used in the European industry: Systema/Outgassing (1) and COMOVA (2). The first tool is known for its agility to model and easiness to analyse a spacecraft whereas COMOVA contains an impressive amount of physical models. Both software have the same numerical core. Nevertheless, it often happens that the same analysis performed with the two tools shows discrepancies. This creates some confusion since some satellite primes use the first one and others the second.

To deal with this situation, OHB performed a full numerical comparison between the two tools. This article summarizes this work that should give more confidence to all the parties in our two European software.

NUMERICAL MODELLING

This section is summarizing the different numerical methods used by both tools so it gives a general view about the capabilities available to model the outgassing phenomena.

All of these information and descriptions in this section are extracted and compiled from Systema (1) and COMOVA (2) user manuals.

The computation of contaminants on surfaces as function of time is performed via two main steps: computation of mass transfer factors and calculation of the mass deposits.

1.1 Mass transfer factors: view factors and ray tracing quality

Molecules are transported through several ways: by direct flux and reflection, under atmospheric flow or due to self-scattering. The Mass transfer factors involve the geometry, atmospheric density and relative velocity, the contaminant density around spacecraft and the molecule properties. When there is no molecule scattering, only spacecraft geometry is involved, reducing the mass transfer factor to the classical view factor from *i* to *j*.

In Systema, the computation assumes that the flow is rarefied and view factors are only determined from surface to surface.

COMOVA deals with four types of view factors: the classical view factor F_{ij} (from surface to surface) by direct line-of-sight transport, the line-of-sight surface to volume VFs (V_{ij}), the volume to surface view factors (H_{ij}) and lastly the VFs from volume to volume (G_{ij}) (when collisions need to be modelled).

$$F_{i,j} = \frac{mass\ emitted\ by\ i, reaching\ j}{mass\ emitted\ by\ i}$$

$$F_{ij} = \frac{1}{S_i}\int \frac{d^2S_i d^2S_j cos\theta_i cos\theta_j}{\pi r^2}$$

Rays are emitted in a random way from the surfaces in order to determine where the outgassed species will deposit. The view factors are stored in a matrix. This matrix can be symmetrised by coupling the nodes. This option can be deactivated for both software's. Which way is chosen might influences the mass conservation. Mass can be lost when rays are impinging inactive sides.

The quality of ray-tracing greatly influences the results. Knowing where the rays come from and where they go can tell whether the deposit comes directly from a surface or is due to reemission.

In Systema V4, in addition to all the model nodes, three extra nodes give to the user a good idea about the quality of his meshing and ray-tracing.

The "Space" node that surrounds the geometry allow to investigate how much contaminant is outgassed to space, since all rays going to space are intersected by this single space node. In addition, "VF imbalance" node and "Inactive Impingements" node show what percentage of rays get lost.

On the other hand, COMOVA does not have the option to look into the view factors. The only way to determine whether enough rays are emitted from all surfaces is by checking convergence. This is done by releasing more and more rays until the results do not change within a certain percentage. However, COMOVA contains a face called '0' that represents space.

Ray-tracing quality is important since some rays can impinge inactive surfaces and therefore, mass conservation is not insured. Both software allows the user to check the mass conservation (through the node 0 and the total deposited mass).

1.2 Mass deposit: Emission, Reemission, Reflections and sticking

The numerical modelling of the mass deposit is closely linked to our physical understanding of the phenomena.

First, the mass deposit depends on the mass flow rate $\dot{W}_e$ that takes into account the emitter mass flux $\dot{W}_{e,k}$.of a species k.

$$\dot{W}_e = \sum_{k=1}^{NE} \dot{W}_{e,k}$$

The emitter mass flux $\dot{W}_{e,k}$.is function of the residence time $\tau_{e,k}$ and follow a first order law to model mainly the desorption. This approach makes the assumption that the desorption is the main mechanism whereas the diffusion is neglected.

$$\dot{W}_{e,k} = \frac{W_{e,k}}{\tau_{e,k}}$$

The first model used for the species emission is the linearized exponential (ESTEC) that consider each species as mathematical one (3) with its own residence time at a reference temperature and thickness $\tau_{e,k}(T_0, h_0)$. The empirical coefficient K_e for temperature effect is common to all species.

$$\tau_{e,k}(T,h) = \tau_{e,k}(T_0,h_0)\left(\frac{h}{h_0}\right)^2 e^{K_e(T-T_0)}$$

The second model is based on Arrhenius Law that considers the residence time as a function of the activation energy E and the materials temperature T.

$$\tau_{e,k} = A^{-1}e^{\frac{E}{RT}}$$

In both cases, the residence time is extracted from a specific testing where the material is heated through different temperature plateaux.

Reemission is based on the same model as the emission and also assumed to follow a first order desorption law. Reemission is complicated to measure in a test up due to that fact that molecules need to be reemitted from the TQCM and captured again.

ESTEC ECSS (3) recommends a crude approximation for reemission by setting the reemission time at temperature T to the emission time constant at $T + 50$ K. This was done considering that reemission was faster than outgassing. This approach shows limitations since in this case, sticking and reflections are not considered.

However, it is known that outgassing, in its complexity, is a competition between desorption and diffusion, reemission, sticking and reflections.

Sticking can be seen as a coefficient that is used to model slow or fast reemissions. When the reemission time of a species is very small, sticking can be set to 0. Reemission will then be considered as a reflection (less computation time). On the other hand, at short times scales, other species will not reemit and thus a large fraction will stick. Then the sticking can be put to 1, so that reemission is not taken into account in the calculation.

For Systema, sticking is not modelled. In case all deposit needs to be captured, the surface temperature is set to 0 Kelvin.

For COMOVA, concerning condensation, a sticking coefficient $S^k(T)$ is defined as a function of temperature:

$$S^k(T) = \frac{1}{2}\left(1 - tanh\left(\frac{T - T_c^k}{2\Delta T_c^k}\right)\right) = \frac{1}{1 + e^{\frac{T-T_c}{\Delta T_c}}}$$

T^k_c is the capitation temperature for species k. The difficulty here is to determine the captation temperature. Until today, it is complicated to determine this capitation temperature through an appropriate testing.

The reflection coefficient is complementary to the sticking coefficient, thus R = 1 – S. The part that does not stick will be reflected. Reflections do not have to occur immediately, they depend on the reemission times. In case the reemission time is shorter than the calculation time step, the reemission process will be replaced by direct reflections in COMOVA. Reflections are handled in COMOVA by matrix multiplication.

Systema does not take into account reflection but model the contamination molecules as travelling from one surface to another via a ray it will stay a certain time on that surface. The time is determined by the reemission parameters. As soon it reemits, a new path is created. This process repeats during the entire mission time.

COMPARISON CASES

Several cases were set-up to extensively compare both software. The idea is to numerically test each feature and compare it to test data when available.

First, a simple case was modelled where two plates are parallel, one contains the outgassing material and the second one is the receiving entity. An analytical solution is available in this case.

Then, the ESTEC set-up, a closed cavity, was modelled for the PU1 paint with different temperature variation. This case was used to compare the reemission and the full reflection models.

Finally, a spacecraft model was computed with both numerical tools.

2.1 Simple case: two plates

The simple case consists of two identical plates of 1 x 4 m are that are placed parallel to each other as shown in Figure 1. The distance between the plates is 1 m.

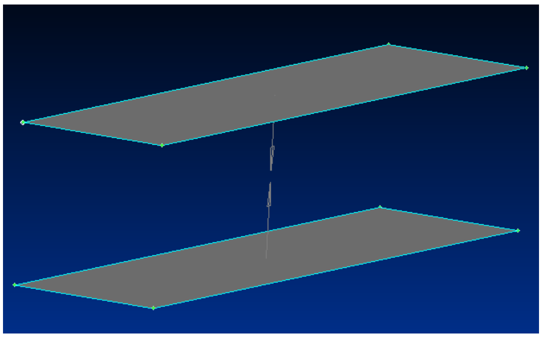

Fig. 1. Simple case set-up

This case was chosen since the view factor can be determined analytically as explained in (4). Ray tracing is tested through launching several number of rays for both numerical tools from 10 rays to 10^6 rays with step factor of 10. Convergence is checked by determining the relative error between the results of the simulation and the analytical value. The second plate has a temperature of 0K in order to capture all deposit.

The relative error between the view factors from the simulation and the analytical values are shown in Table 1. This table presents only the VF from plate 1 to 2 and for various number of rays as explained in the previous paragraph. The comparison for the inverse view factor showed also the same trend.

Obviously, the more rays are launched the better are the results. The same behaviour is observed and acceptable convergence is reached since the relative error is within 3 % for 10.000 rays and within 0.5% for 10^6 rays.

Number of rays	Systema (%)	COMOVA (%)
10	**71%**	**42%**
100	9,8%	13%
1.000	5,5%	4,3%
10.000	0,06%	2,2%
100.000	0,65%	0,22%
1.000.000	0,34%	0,27%
10.000.000	**0,14%**	**0,25%**

Table 1. View factors comparison: Systema and COMOVA vs Analytical solution

In addition, both tools have an option to symmetrize the view factor matrix. Symmetrizing the matrix can be use in cases where the model is somehow equilibrated in terms of geometrical elements size. This option could however lead to mass loss and mass conservation issues.

The two tools are again in line with each other's when the view factors are calculated with and without the symmetry option. The mass conservation is conserved whether 10 rays are launched or 10^6 rays. The error is just in order of 10^{-13} kg (it can be considered negligible). When the symmetry is activated, it can lead to a conservation issue for both tools.

10 rays	**Systema**	**COMOVA**
F12	-2.60E-13	9.00E-12
F12 Symetry	6.33E-07	-2.00E-06
10^6 rays	**Systema**	**COMOVA**
F12	6.40E-13	6.00E-13
F12 Symetry	1.05E-10	7.00E-10

Table 2. Mass conservation: Systema vs Comova

When plotted, the curves are perfectly in line in the 10^6 rays case.

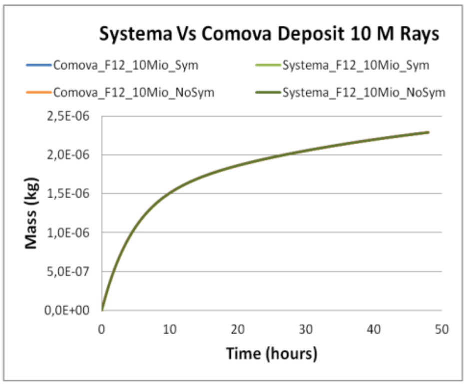

Fig. 3. Systema vs Comova deposit evolution in the simple case

This first case give a first indication about the behaviour of the two tools with regard to an analytical case. The ray-tracing module for both is stable and in line with each other's.

2.2 ESTEC VBQC Test Chamber

ESTEC VBQC Test chamber consists of two cylindrical chambers connected by a tube. There is no direct line of sight between the sample and the QCMs due to a narrowing at the entrance of the cold chamber (5).

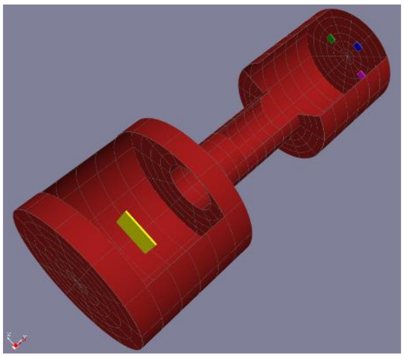

Fig. 2. ESTEC VBQC Test Chamber set-up

The test set-up is as follow: the sample containing an outgassing material is heated in one chamber. The walls of the second chamber are kept at liquid nitrogen temperature (0.1 K simulations). Three QCMs are placed at a wall of the cold chamber.

Numerous cases were simulated to study the effect of the temperature on the outgassing experiment that lasts 120 hours. The first case is the "standard" test performed is a multi-step temperature test where the sample temperature is increased from 25 °C to 125 °C by steps of 25 °C every 24 hours. The QCMs are at -150°C, -100°C and -50°C. The first case results was already validated for COMOVA and its results can be found in (5).

The "reflections" case is done by setting the walls temperatures to 25 °C (0 sticking in COMOVA). The QCMs have a temperature -273°C in order to capture all contaminant. This set-up determines the difference between using reflections in COMOVA and purely reemission in Systema.

The second case shows the importance of the reflection in comparison to the reemission. COMOVA is perfectly modelling the test set-up thanks to the reflections and no sticking whereas Systema can only rely on reemission approach. In the Systema case, the deposit reaches only half of the maximum deposit at the 120 hours.

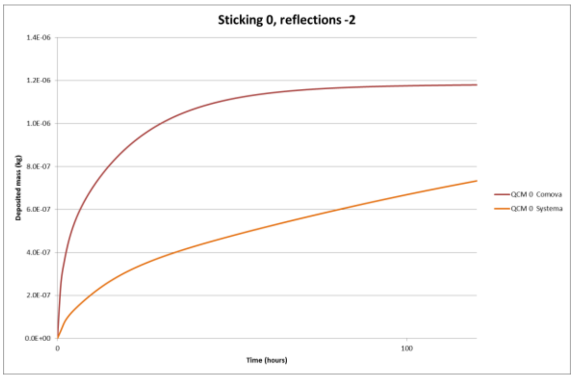

Fig. 4. Systema vs Comova deposit evolution for the ESTEC "full reflection" case

This result can be due to mass conservation issues inside the cavities nevertheless it is solely related to the absence of reflection in the Systema model. In fact, by extending Systema to 1200 hours, the maximum deposit is also reached. This could mean that the reemission approach is insufficient to model a closed cavity.

Fig. 5. Systema elongated simulation

As specified earlier, the reemission approach chosen by ECSS is to take the emission times and to add 50K to the temperature. This crude approach could be however enhanced by correlating reemission and reflection approaches. In fact, this case is a perfect example to check the possibility of choosing a better reemission time residence for each species.

The first method is to start from the formula of the mass deposit that is obtained with linking the residence time to the deposit.

$$m_{deposit}\left(t,T,T_{QCM}\right) = m_0(1 - e^{\frac{-t}{\tau e^{-K(T-T_0)}}})$$

In this case, the temperature is equal to the reference case which simplified the precedent equation to:

$$m_{deposit} = m_0(1 - e^{\frac{-t}{\tau}})$$

To link the reemission to the reflection, the final deposit obtained with the reflection case can be used to deduce the time needed to reach the asymptote.

This gives the new reemission residence time dependency on the initial deposit and refection time.

$$\tau_{r)node} = \ln(1 - \frac{m_{Reflexion}}{m_0})t_{reflexion}$$

In the ESTEC case, the QCM is not in direct view with the contaminating sample, therefore, the view factor $VF_{average}$ from all the nodes can be taken into account to include the geometrical properties of the ESTEC chamber.

$$\tau_{r)all} = \ln(1 - \frac{m_{Reflexion}}{m_0})t_{reflexion}\, VF_{average}$$

With COMOVA simulation, this reflection time can be extracted as well as the average view factor since the reemission depends on the view factors between surfaces.

The second method is to find a better temperature correlation between the reemission and the emission residence time. This can be done empirically.

Applied to our case, the two methods provide the following results for the first three species:

	Reemission residence time (h)		
Species	**ECSS**	**Full Reflection model**	**Temperature translation (+100K)**
PU_1_A	1.20E-03	1.60E-04	1.20E-04
PU_1_B	1.20E-02	7.37E-04	1.20E-03
PU_1_C	1.2E-01	1.40E-03	1.20E-02

Table 2. Mass conservation: Systema vs Comova

When these residence time were applied to Systema calculation the following results were obtained.

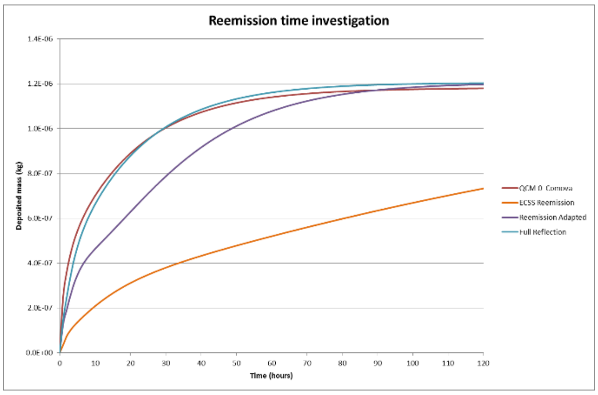

Fig. 6. Reemission time investigation.

This investigation showed that there is a possibility to adapt reemission time to better fit experimental data for a closed cavity. The ECSS approach is completely off in this case and cannot be adapted. The mathematical model obtained by OHB can be actually used to better fit the reemission time to the reflection one. It appears that a 100K translation can be a good first approximation

2.3 Spacecraft semi open cavity

The comparison between the two software has also been performed for a spacecraft case with a sensitive item being a semi-closed cavity.

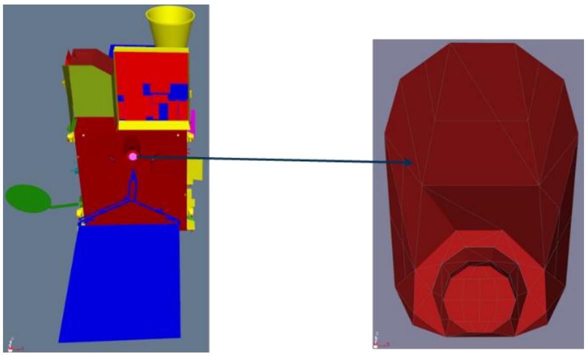

Fig. 7. Semi-closed cavity case

The Kapton material can outgass on the internal lens of the sensitive item. The spacecraft is on a geostationary orbit (no atmosphere) and the temperature is considered constant in this case.

First approach of the simulation was using sticking and infinite reflection for COMOVA and only reemission for Systema. The result showed a huge discrepancy between the two approaches. The maximum deposit in kg/m² is around 1E-11 in one case and 1E-07 in the second case.

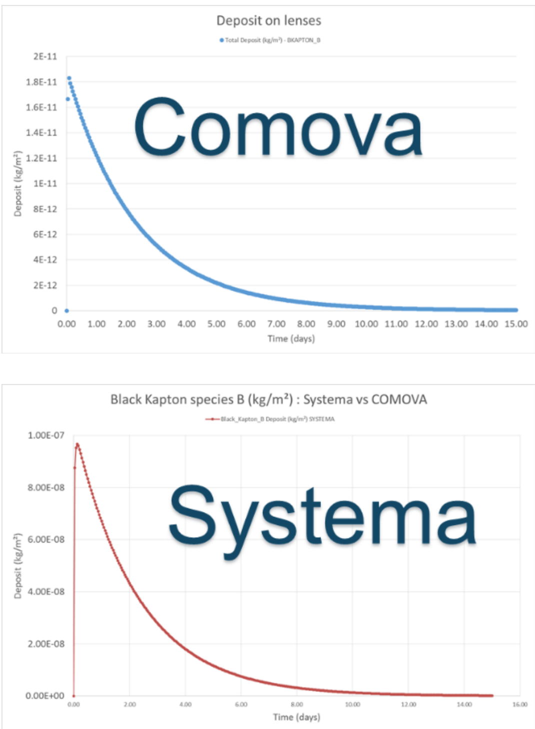

Fig. 8. Two tools discrepancy

This is mainly due to the fact that the sticking coefficient in COMOVA plays a role as seen in the Fig 8. By adapting the condensation temperature to set the sticking coefficient to 1, the reemission process could take place in COMOVA.

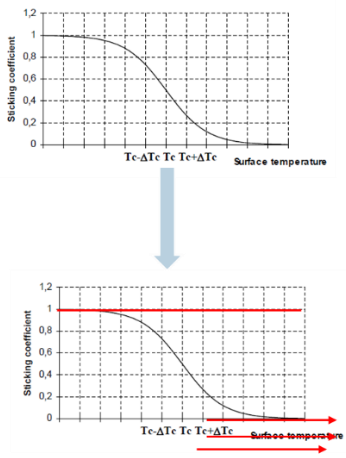

Fig. 9. Sticking coefficient adaptation for COMOVA

The following results were obtained and the tools were again in line.

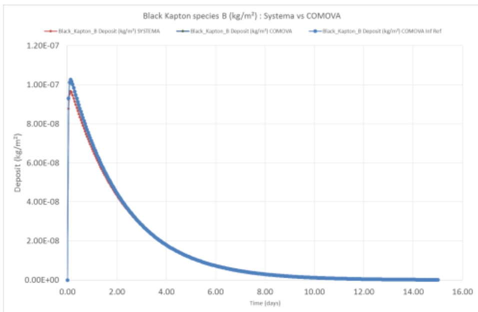

Fig. 10. Sticking coefficient adaptation for COMOVA

The spatial distribution is perfect between Systema and COMOVA (displayed in FEMAP) which means that the results converged in terms of ray distribution. Therefore, the consistency between the two tools are here demonstrated.

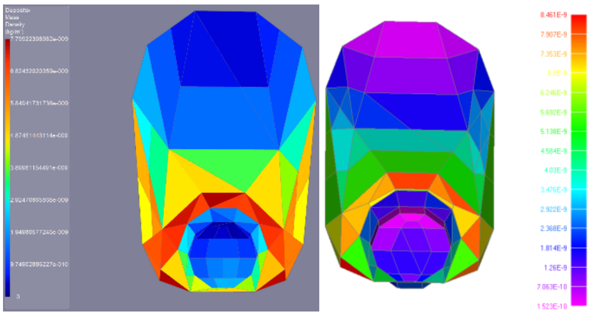

Fig. 11. Spatial distribution of the deposit obtained with the two tools: Systema (left) and COMOVA (right)

However, this analysis asks us a real question: which one of the two approaches is physically correct? Full sticking and only reemission? Or the "classic" sticking approach of COMOVA is the correct one?

CONCLUSION AND PROPOSITION OF SIMULATION GUIDELINES TO THE COMMUNITY

This article summarizes the work done for comparing the two tools. The main conclusion is that the two tools are perfectly in line when it comes to model numerically the contamination.

The two software have the same numerical core for the ray-tracing and are converging reasonably for all observed cases. Systema model the reemission as specified in the ECSS guideline and COMOVA have more options to take into account the reflection phenomena and the sticking coefficient.

In this paper, a tentative was elaborated to link reemission residence time to the reflection approach. This showed that the ECSS guideline is misleading and can lead to issues in the final deposit. Both of the software rely on the state-of-art modelling progress in this field. It is important to state that more effort need to be done to better characterize the outgassing.

In the Bremen workshop, the idea of a guideline to the users was proposed. In this article, a quite generic guideline proposal is made that can further evolve with the inputs from the community:

A. Ray-tracing:
   - A.1. According to the first case, convergence was obtained starting from 10.000 rays for one node. This number is a minimum for an emitting node.
   - A.2. If a ray impinge a non-active face, a mass conservation issue can happen. In addition to checking model geometry in both software, one have to check Systema Space node and Comova face 0.
   - A.3. Symmetry option can be used in the case of a balanced model. Otherwise, this option has to be avoided.

B. Mass deposit
   - B.1. Reemission parameters need to be adapted. For a closed cavity, an adaptation of the reemission temperature is needed (+100K) for Systema whereas infinity reflection are the best parameter choice for COMOVA
   - B.2. Sticking coefficient has to be carefully used in COMOVA until further investigation is carried out with more test data.
   - B.3. No particular issue was observed for the integration time step for both software. However, a special care has to be given for fast species modelling with Systema.

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