Advanced web tools for promoting the application of nanotechnology and the safe use of nanomaterials in the plastic sector

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LIST OF ACRONYMS

ENM	Engineered nanomaterial
FF	Far field
NMs	Nanomaterials
NF	Near Field

EXECUTIVE SUMMARY

In task 4 of the NanoDESK project, the goal is to design a model predicting the fate and transport of the airborne ENMs in workplaces released from processes related to the plastic sector. Several current models were revised and properties of the ENMs analyzed to predict their influence and relevance on the risk of emission.

The occupational model was mathematically developed and coded in Python. Several performance tests were completed to analyze the scope of the model and a pre-design of the layout to be implemented in the tool repository of the NanoDESK platform was drafted.

In the following document, a detailed description of the steps followed and the basis of the model are depicted.

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1. Scope and objectives

The development and commercialization of products and technologies that use nanomaterials entails the need for proper risk management and to assess the potential for exposure to these new materials throughout their life cycle. The possible routes of exposure (inhalation, dermal and oral) are very different between them and objects of many studies, as well as the complex processes of transformation, the characterization and comprehensive understanding of the exposure is still a distant goal. Some of the challenges to face, according to (1) and (2) are:

1) **Metric**: While traditionally mass has been the choice in the case of materials in primary form, when we face the measurement of nanomaterials becomes almost negligible parameter, therefore other physical-chemical properties, such as shape, size, solubility or reaction surface are on debate on the most appropriate metric to describe the " effective biological dose "
2) **Instrumental limitations**: measuring the physical-chemical properties mentioned above is still a very complex task. Existing instruments use different physical principles and are not able to collect all the necessary information, requiring the use of a combination of different equipment with the intention of obtaining a complete profile of a given aerosol;
3) **Background**: its contribution to the concentration of nanoparticles is fundamental to understand their influence on the measurements carried out in order to evaluate the exposure. This fund is generated by different sources, which can be natural (such as volcanoes, for example) or artificial (which combustion and accidental release of ENMs).
4) **Spatial and temporal profile of the aerosol**: the concentration of ENMs can be influenced by an enormous number of factors related to the location (for example, the phenomena of agglomeration and aggregation very close to a source, where the concentration is higher) as over time. The behavior of the substances in the presence of these environmental factors is of extreme importance and that is why multiple measurement campaigns are recommended and a meticulous record of conditions such as humidity and temperature.

In order to overcome all these difficulties, a practical and multifaceted strategy is necessary. Mathematical models for estimating exposure can be used to simulate the emission of a source and transport in the work environment, as well as in the different compartments of the environment (air, water, sediment, soil, etc.). It has been demonstrated in recent years that models, as well as direct measurements, can be used in general for the evaluation of exposure, and a large number of tools have already been developed. The use of some of them is suggested by ECHA in their technical guides (3,4) and others are currently in the process of validation. However, when the models for existing chemical substances are applied to nanomaterials, serious difficulties arise due to the rapid changes in aerosol nanoparticles, for example, due to different processes, such as agglomeration, coagulation, aggregation, deposition, chemical reactions and possible interactions with the background. Despite this, the application of models continues to be a promising path for the development of an exploratory risk assessment strategy.

2. Methodology

The selection of the information required and the parameters needed is based on a thorough analysis of existing models and tools for occupational risk assessment, such as ART (5), Stoffenmanager Nano (6), GuideNano (7) or NanoSafer (8) models.

It is intended as an easy-to-use tool practical for all the stakeholders involved: expert or not, which is based on very direct and simple questions. Most of them have a multiple selection list to choose from in a quantitative way. The user is guided in every moment through the phases of the evaluation. Default values are used when the user cannot answer to some question.

2.1. Exposure determinants

Due to the lack of reliable and consistent collected exposure data to NMs and the difficulties exposed above, the scientific basis for validation of the existing exposure models is missing or limited. Despite the multiple parameters involved, there have been several studies (9,10) performed in controlled conditions to gain more insight into the effect of various determinants underlying the potential on the concentration of airborne NMs close to the source with the purpose of providing a scientific basis for existing and future exposure inhalation models. A combination of physico-chemical characteristics of the substance, which can be influenced by the process itself, the operative conditions and the risk management measures in place, could lead to different results for the same nanomaterial.

However, these works have probed that some parameters have a greater degree of influence in the release and spread of NMs than others. For example, it seems that particle surface coating did not affect the number concentration of released NMs, but an increase of the powder's moisture content resulted in less and smaller particles in the air (9).

Latest researches (11,12) indicate that the main factors affecting emission potential in the near field are the type of source (continuous, intermittent) and ventilation rate with smaller, nearly negligible differences between the NF and FF concentration when the ventilation rate is set to very low volumes, while deposition and aggregation do not play a significant role since there are no substantial differences on the size distribution on the NF-FF. In this sense, for a constant source and fast or slow mixing, the two-box model will provide an accurate estimation of the concentration, even could be simplified to a 1-box model for very low rates.

Considering these characteristics, the following determinant parameters have been considered and its influence pondered to achieve closest to reality results. They have been classified depending upon nanomaterial characteristics, process characteristics or conditioning of the room:

2.1.1. Nanomaterial characteristics:

Related to the substance intrinsic characteristics, it has been found determinant:

- **State of the substance:** the NanoDESK Occupational Exposure Model includes two possible states of the substance:

- *Solid:* intended as a powder if we are considering a process where raw material is handled, like synthesis or formulation, as well as a powder already embedded in a polymeric matrix undergoing an activity that could generate airborne dust.
- *Liquid:* intended as a liquid suspension undergoing a process that could lead to aerosolization.

The parameters taken into account are not the same for the two possible states of the nano-enabled material. In particular, in the case of liquids, dustiness will not play a role. On the other hand, viscosity and volatility will not be considered when dealing with solids.

PHYSICAL STATE	• Solid • Liquid

- **Dustiness**

It can be considered as **the key parameter for the intrinsic emission potential of a solid** (13) and describes the tendency of a substance to generate airborne particles. It is not only related to the physical form of the substance but also to the electrostatic forces between the particles. It can be influenced by bulk density, shape, size and length and it is strongly dependent on whether the nanomaterial is in powder form or incorporated into the polymeric matrix. Dry powders pose the highest risk of inhalation exposure, which diminishes drastically when the substance is incorporated in a paste or a solid due to the limited mobility at least as long as the matrix stays unbroken. It is not yet possible to quantitatively assign a dustiness level to a substance, such that in exposure assessment it is usually assigned a class to the substance. For example, in the case of the Advanced Reach Tool (ART) (5), there are six possible classes: firm solids, firm granules or flakes, granules or flakes, coarse dust, fine dust and extremely fine dust. The dustiness of commercially available nanomaterials is usually low but there exist exceptions, as it is the case for carbon nanotubes, which span a very wide range of dustiness classes. For example, in (9) it was found that dumping of nanopowders resulted in a higher number concentration and larger particles than dumping their reference microsized powder ($P < 0.05$). Furthermore, the results indicate that particle number concentration increases with increasing dump height, rate, and mass and decreases when ventilation is turned on.

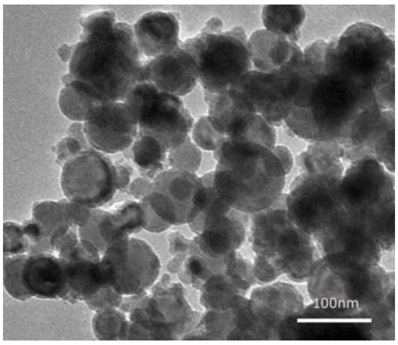

Figure 2: Copper nanoparticles.

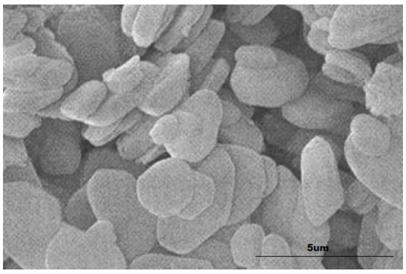

Figure 1: Graphite nanoflakes.

DUSTINESS	• Very high (extremely fine and light powder) • High (fine powder) • Medium (coarse powder) • Low • Unknown

- **Solubility**

Solubility is a key factor to determine the hazardousness of a nanomaterial, because it is determinant for its biopersistence and biokinetics. An insoluble or slightly soluble nanomaterial will have the opportunity to be transported from the entry point in the body (lungs, gastrointestinal tract, skin, nose) to another compartment (translocation) to be redistributed in other organs and tissues (accumulation). If other factors hinder its transport, the accumulation may occur in the same place of entry. In both cases, the accumulation in a site increases the risk of chronic adverse effects. On the other hand, the tendency is to treat an insoluble substance as an ordinary toxicological problem (14).

SOLUBITILY	• Yes • No • Unknown

- **Weight fraction / Dilution**

Since the purer is a substance (100% nanomaterial), the higher the probability of exposure, it has been adopted the same assumption to the base of the ART model (5); the emission of a solid resulting from the activity is linearly related to the weight fraction of the ENM. The same will be valid for dilution in the case of a liquid.

WEIGHT FRACTION / DILUTION	• > 99 % • 50 – 99 % • 10 – 50 % • 1 – 10 % • 0,01 – 1 % • < 0,01 %

- **Moisture level**

As commented previously, increasing the humidity level or adding additives to a solid object before a process begins, the emission potential is reduced due to the layer of liquid on the surface of the particles that increases the forces between them.

MOISTURE	• Dry (< 5%) • 5-10% • > 10%

- **Viscosity**

Viscosity is a key parameter for the evaluation of exposure due to a liquid substance. Molecules of products with high viscosity, such as resins or adhesives, are bonded with greater force, making the release of nanoparticles by aerosolization less likely. In this regard, the vapor pressure It is critical to determine the ease with which molecules can be released from the surface in contact with air.

VISCOSITY	• Low (like water) • Average (like oil) • High (like pasta, syrup)

- **Shape of substance**

Geometrical shape of the substance will also determine the effects that the entrance of the nanomaterials to the body organs may have. For example, nanotubes are known to cause pulmonary inflammation and have effects similar to asbestos

SHAPE	• Dust • Fragile granules / flakes • Firm granules / flakes • Fibers

- **Amount of substance**

The amount of pure or pristine substance is a fundamental parameter that can be referred to different concepts. While in other models it consists in the daily amount of material used (CB Nanotool (14,15) or Precautionary Matrix (16)), the NanoDESK model, analogously to NanoSafer (8), refers to the amount employed in each task of the work cycle.

AMOUNT	• ___ g/h • ___ kg/day • ___ tons/year

2.1.2. Process characteristics:

On the other hand, regarding to the external (ambient and process related) conditions, the highlighted determinants are:

- **Energy of the Process/Activity**

The emission potential is directly related to the activity and depends on the energy applied to the process: during a more dynamic process, nanoparticles are more likely to be released. It is one of the most important parameters, since can modify the influence of the other physico-chemical characteristics in the final emission rate.

ENERGY OF THE PROCESS / ACTIVITY	• High: *mechanical mixing at high speed, pouring the product from big bags, spraying products using high pressure or spray paint, boiling liquids, mixing products at high speed* • Medium: *manual pouches of bags, mechanical mixing at low speed, quick dives and without care, aeration tanks, electroplating* • Low: *precise, slow and controlled dives, mixing or manual sieving of the product*

- **Duration of the activity/pause**

Understood as the duration of each of the activities or tasks that make up the entire work cycle, including the pause between cycles and the number of repetitions. In this way, both intermittent or constant sources are covered.

DURATION OF THE ACTIVITY	• Constant • Intermittent regular • Intermittent irregular

2.1.3. Facility characteristics:

- **Background concentration**

Will help to discern the number of nanomaterials that are released from the source during a certain process from the basic number of particles in air when no task is being carried out, due to natural conditions, neighbor processes or incidental release.

BACKGROUND CONCENTRATION	• Indoors without activity • Indoors with activity without ENMs • Outdoors

- **Volume of the facility**

While the volume of the NF is assumed to be fixed and equal to 8 m^3, the volume of the FF is that of the rest of the room. Therefore, the residence time of the particles and thus the compartmentation of the model selected will be different depending on the size of the installation.

VOLUME OF THE FACILITY	• < 10 m^3 • < 10-100 m^3 • < 100-1000 m^3 • > 1000 m^3

- **Ventilation rate**

It refers to the general ventilation system present in the installation, i.e. the air flow that is transported from the FF to the outside of the installation. As is stated in (12), it is one of the most determinant parameters to determine levels of exposure. It has been considered plain general ventilation and with recirculation and/or filtration.

VENTILATION RATE	• < 0,5 m/s • 0,5 – 1,0 m/s • 1,0 – 2,5 m/s • 2,5 – 10 m/s • > 10 m/s

- **Climatic conditions**

  The temperature and humidity levels inside the installation has a significant impact on the levels of exposure to particles with size in the nano range, due to its influence on phenomena such as agglomeration and aggregation. A high degree of relative humidity will propitiate the agglomeration/aggregation, while high temperatures can promote the nucleation or release from other sources.

CLIMATIC CONDITIONS	• T = ____ ºC • RH = ____ % • P = ___ bar

- **Risk Management Measures (LEV)**

  The ventilation near the source, in the NF and the interchange of air between NF-FF is strongly influenced by the presence of ventilation systems. If this flow is low, the exposure in the NF will be significantly higher, while increasing it, the exposure level of the NF will decrease and will have the same order of magnitude as in the FF. In this case, we have considered several options considering the general ventilation with or without the recirculation, plus the ventilation rate and the efficiency of the LEV in place, also with or without recirculation and filtration of the extracted air, as it is developed in (17).

LOCAL EXHAUST VENTILATION TYPE (LEV)	• Integrated (in machine or tool) • Cabin • Fume hood • Side hood • Suspended hood • Other • None

- **Filtration type**

  Along with the type of LEV applied, the facility may have general ventilation or local ventilation with different types and efficiencies of filter systems, which will determine the model selected.

FILTRATION TYPE	• HEPA • ULPA • Other • None

In view of the above parameters, a mathematical model has been constructed that forecasts the emission of nanoparticles in an occupational scenario.

2.2. Mathematical model

The NanoDESK model for the estimation of occupational exposure to ENMs relies on the **near field/far field (NF/FF) source receptor approach** proposed for the first time by Cherrie et al (10,18) and it is based on the model recently developed by Tsang *et al.* (19). The source receptor model consists in a very simple theoretical model widely used to evaluate or predict exposure levels, composed by a source term dependent on the intrinsic properties of the contaminant and responsible for the emissions which disperse away from the source. Such factors comprise the parameters describing the physico-chemical properties of the nanomaterial mentioned in the previous section, such as dustiness and moisture level, as well as the amount of substance employed. This dispersion is simplified introducing two special concepts:

- **Near Field (NF)**: which is the part of the volume of the room containing the source and the worker exposed to the contaminant;
- **Far Field (FF)**: which is the rest of the work environment.

The model can work indistinctly with mass or particle number concentrations, considering the appropriate conversion factors. For simplicity reasons, and since it is the original parameter used in the development of the models, only mass related parameters will be presented here. Four basic assumptions underlie the model:

1) all the mass of contaminant involved is generated by the source in the NF volume and quantified by an emission potential we call E_s with units of kg/s;
2) the air flow between the NF and the FF zone is limited and given by a factor β with units of m^3/s;
3) in both the NF and FF volumes the concentrations are homogeneously mixed;
4) the only loss of contaminant is due to the FF general ventilation, whose flow we will call Q and which has units of m^3/s.

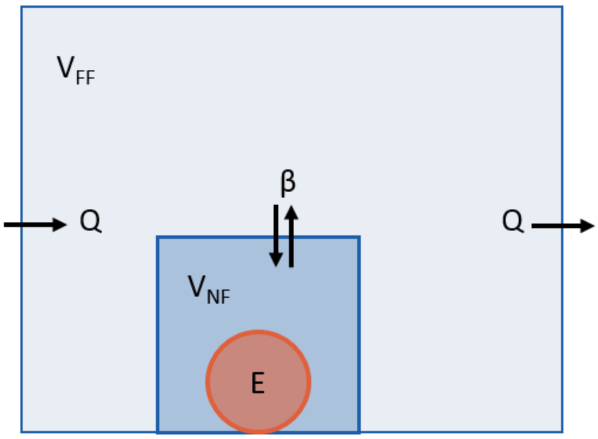

Figure 3: Schematic representation of the NF/FF approach used to build the model.

The situation described above is schematically represented in Figure 3 and defined by the two mass balance equations for the NF and FF concentrations written below:

$$V_{NF}\frac{dC_{NF}}{dt}(t) = E_S(t) + \beta C_{FF}(t) - \beta C_{NF}(t) \quad (1)$$
$$V_{FF}\frac{dC_{FF}}{dt}(t) = \beta C_{NF}(t) - (\beta + Q)C_{FF}(t) \quad (2).$$

In Eqs. (1) and (2) C_{NF} and C_{FF} are the concentration of the contaminant in the NF and in the FF volumes measured in mg/m^3, V_{NF} and V_{FF} are the NF and FF volumes (m^3) and t is the time (s). As already mentioned, the factor β (m^3/s) is the NF-FF air flow, while Q (m^3/s) is the ventilation flow of the FF, which as will be seen in the following, will depend on the ventilation controls present.

The emission potential E_s (mg/s) is defined as:

$$E_S = \frac{dm}{dt} \cdot R \cdot EHP\,, \quad (3)$$

where *dm/dt* is the mass flow which can be approximated as constant rate as:

$$\frac{dm}{dt} = \frac{\Delta M}{\Delta t} \cdot wt\ (\%), \quad (4)$$

with *ΔM* being the amount of substance employed in the activity, *wt* (%) is the weight fraction of the total substance that is pristine nanomaterial and *Δt* the task duration. This is equivalent to assuming that in a given time interval it is employed in the activity a constant amount of substance.

The factor *EHP* in Eq. (3) refers to Energy Handling Potential, and it is a factor between 0 and 1 that defines the amount of potentially released material depending on the energy applied to the mass of nanomaterial in different ways: temperature, potential energy, pressure, velocity, etc.

The factor *R* in Eq. (3) is a factor determining which fraction of the mass flow is being emitted by the source. The emissions, as already mentioned at the beginning of this section, depend on the characteristics of the source. In particular, it was taken into account different factors depending on the solid or liquid state of the product:

$$R_{sol} = w_1 S + w_2 D + w_3 W, \quad (5)$$

$$R_{liq} = w_1 S + w_2 V + w_3 Sol \quad (6)$$

In equations (5) and (6), S is the physical state of the substance, if solid or liquid. In the case of solids, *D* is the dustiness and *H* the moisture level of the solid; while in the case of liquids, *V* is the volatility or the vapor pressure and *Sol* the solubility in water. The factors w_1, w_2, and w_3 represent the different weights attributed to the determinants, taking values of 0.3, 0.5 and 0.2 respectively.

Therefore, the emission potential E_s to be inserted in Eq. (1) has already accounted for the influence of the physico-chemical characteristics of the substance and the process.

The initial background concentrations present in the room can be estimated supposing steady state in the place. The steady state assumes that generation rate is constant and that sufficient time has elapsed so that the contaminate mass leaving the system via the room exhaust is exactly balanced by the mass being released

$$C_{NF}(0) = C_{FF}(0) + E_S(0)/\beta \quad (7)$$

$$C_{FF}(0) = E_S(0)/Q \quad (8)$$

(20). The initial concentrations can be calculated therefore from an estimate of the generation rate and the ventilation rate:

The flowrates between NF-FF and FF to the exterior are influenced by the types of risk management measures. Several cases are considered:

- **V1: Only General Ventilation.** Natural or general ventilation homogeneously distributed through the room, with exhaust to the exterior of the room.
- **V2: General Ventilation + Recirculation & Filtration.** This is the case when the air of the previous case is returned to the room after filtration process. In this case, it has to be taken into account the room recirculation ventilation rate, Q_R, and its filtration efficiency, ε_{RF}.
- **V3: General Ventilation + LEV.** This case considers any type of Local Exhaust Ventilation that subtracts a flow rate from the source to an independent exhaust system, including capture hoods, fume hoods, etc. The local exhaust ventilation rate, Q_L, and its efficiency, ε_L, have to be taken into account.
- **V4: General Ventilation + Recirculation & Filtration + LEV.** It is a combination of cases V2 and V3.
- **V5: General Ventilation + LEV with Recirculation & Filtration.** In this case, the general ventilation is as in case V1 but the LEV recirculates the filtered air that provides, therefore, the parameters of case V3 have to be considered plus the filtration efficiency of the LEV filter, ε_{LF}.
- **V6: General Ventilation + Recirculation & Filtration + LEV with Recirculation & Filtration**. It is a combination of cases V2 and V5.

In Table 1 are summarized the values of the parameters to be included in Eqs. (1) and (2) listed in each of the previous cases. Q_0 and β_0 are referred to the plain general ventilation rates to the exterior and between NF-FF respectively (case V1).

Table 1: Matrix of coefficients depending on ventilation type.

	V1	V2	V3	V4	V5	V6
Q	Q_0	$Q_0+\varepsilon_{RF}*Q_R$	Q_0	$Q_0+\varepsilon_{RF}*Q_R$	$Q_0+\varepsilon_{LF}*Q_L$	$Q_0+\varepsilon_{RF}*Q_R$
β	β_0	β_0	β_0+Q_L	β_0+Q_L	β_0+Q_L	β_0+Q_L
Q_L	0	0	Q_L	Q_L	Q_L	Q_L
Q_R	0	Q_R	0	Q_R	0	Q_R
ε_L	0	0	ε_L	ε_L	ε_L	ε_L
ε_{LF}	0	0	0	0	ε_{LF}	ε_{LF}
ε_{RF}	0	ε_{RF}	0	ε_{RF}	0	ε_{RF}

Equations (1) and (2) can be solved analytically as a linear system of equations (i.e., a matrix equation) by finding their eigenvalues and eigenvectors, in this case (20,21):

$$\lambda_1 = 0.5\left[-\frac{\beta V_{FF}+V_{NF}(\beta+Q)}{V_{FF}V_{NF}} + \sqrt{\left(\frac{\beta V_{FF}+V_{NF}(\beta+Q)}{V_{FF}V_{NF}}\right)^2 - 4\frac{\beta Q}{V_{FF}V_{NF}}}\right] \quad (9)$$

$$\lambda_2 = 0.5\left[-\frac{\beta V_{FF}+V_{NF}(\beta+Q)}{V_{FF}V_{NF}} - \sqrt{\left(\frac{\beta V_{FF}+V_{NF}(\beta+Q)}{V_{FF}V_{NF}}\right)^2 - 4\frac{\beta Q}{V_{FF}V_{NF}}}\right] \quad (10)$$

It can be seen the influence of the flowrates in the room in Eqs. (9) and (10), which are determinant to the spread of the NM from the source through the room and therefore, the exposure.

When the emission stops due to finalization or pause between processes, or due to intermittent emission, it is considered the decay phase, where *Es = 0.* Previous mass balance equations are solved analogously.

3. Implementation of the model

3.1. Application of the model

Some examples of the results can be seen in the following. The same case will be implemented with slight variations in each simulation. For example, using as basis a **Case 1** in which it is handled during 1 hour with no pause a mass of 100 g of a dry powdered substance with 90% of purity, not soluble, in a laboratory room of 100 m^3 with natural ventilation of 12 AER/h (ventilation case V1), results can be seen in the following:

TABLE 2: INPUT PARAMETERS CASE 1		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	1	
Ventilation type	v1	only general ventilation
beta	3	m^3/min
Q	20	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 3: MODEL OUTPUT CASE 1				
	Near Field		Far Field	
Steady State mass concentrations:	30,67	mg/m^3	4,00	mg/m^3
Average mass concentrations for the whole cycle:	28,792	mg/m^3	3,489	mg/m^3
Average particle concentrations for the whole cycle:	4,40E+14	#/cm^3	5,33E+13	#/cm^3
8-hour concentration	2,11E+17	#/cm^3	2,56E+16	#/cm^3

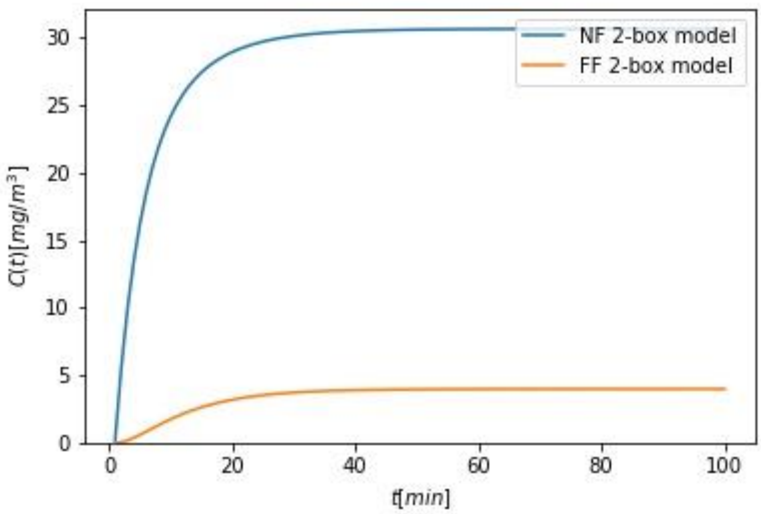

Figure 4: Output concentrations during case 1.

In Figure 4 can be seen the rapid increase of the concentration after the start of the activity and how it remains stable as there is no forced ventilation, background or disturbances during the duration of the activity. Output values are shown in mass and number concentration for comparison. Far field is up to 7 times smaller than the Near field concentration.

Case 2 has the same input parameters expect the total flowrate in the facility is reduced to half, that is 10 m^3/min which corresponds with an AER of 6 h^{-1}:

TABLE 4: INPUT PARAMETERS CASE 2		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	1	
Ventilation type	v1	only general ventilation
beta	3	m^3/min
Q	10	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 5: MODEL OUTPUT CASE 2				
	Near Field		Far Field	
Steady State mass concentrations:	34,67	mg/m^3	8,00	mg/m^3
Average mass concentrations for the whole cycle:	31,443	mg/m^3	6,316	mg/m^3
Average particle concentrations for the whole cycle:	4,80E+14	#/cm^3	9,65E+13	#/cm^3
8-hour concentration	2,31E+17	#/cm^3	4,63E+16	#/cm^3

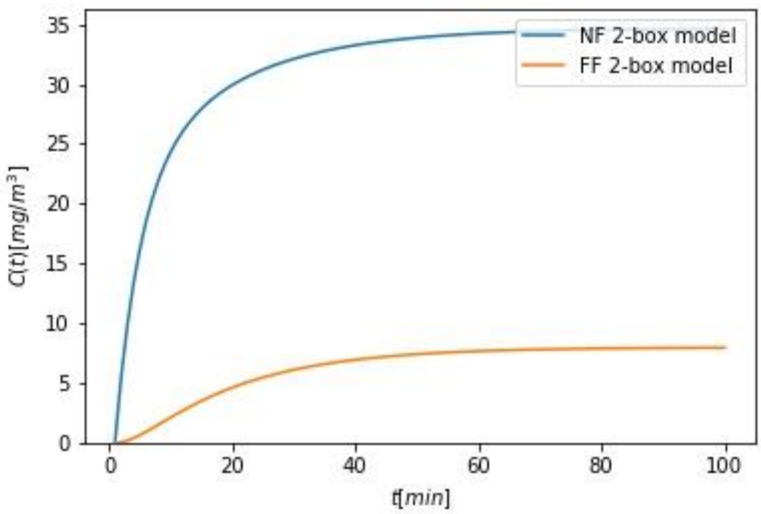

Figure 5: Output concentrations during case 2.

It can be seen in Figure 5 how the increase is slower and slightly greater concentration values are reached in the case of the near field, while in the Far Field is doubled due to the poorer ventilation.

In **Case 3**, the ventilation rate is decreased to reach an Air Exchange Rate (AER) in the room of 1 h^{-1}, showing in Figure 6 no steady state reached and concentrations that double the previous case in the Near Field, but up to 6 times greater in the Far Field, as could be expected.

TABLE 6: INPUT PARAMETERS CASE 3		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	1	
Ventilation type	v1	only general ventilation
beta	3	m^3/min
Q	1,67	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 7: MODEL OUTPUT CASE 3				
	Near Field		Far Field	
Steady State mass concentrations:	74,67	mg/m^3	48	mg/m^3
Average mass concentrations for the whole cycle:	40,615	mg/m^3	16,408	mg/m^3
Average particle concentrations for the whole cycle:	6,21E+11	#/cm^3	2,51E+11	#/cm^3
8-hour concentration	2,98E+14	#/cm^3	1,20E+14	#/cm^3

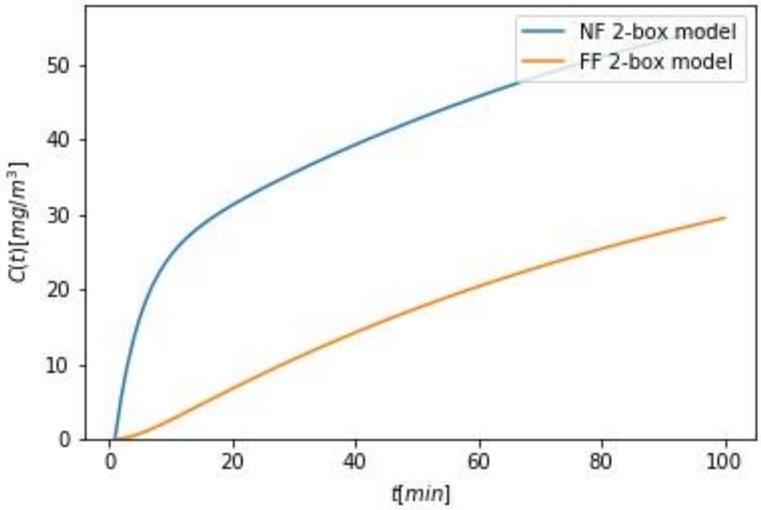

Figure 6: Output concentrations during case 3.

Case 4 is a variation of Case 3 with 3 repetitions of the same activity with no pause in between. It can be seen how each activity increases the concentration in Figure 7, accumulating over the previous one.

TABLE 8: INPUT PARAMETERS CASE 4		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	3	
Ventilation type	v1	only general ventilation
beta	3	m^3/min
Q	1,67	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 9: MODEL OUTPUT CASE 4				
	Near Field		Far Field	
Steady State mass concentrations:	74,67	mg/m^3	48	mg/m^3
Average mass concentrations for the whole cycle:	109,22	mg/m^3	45,92	mg/m^3
Average particle concentrations for the whole cycle:	1,67e+12	#/cm^3	7,02e+11	#/cm^3
8-hour concentration	8,01E+14	#/cm^3	3,37e+14	#/cm^3

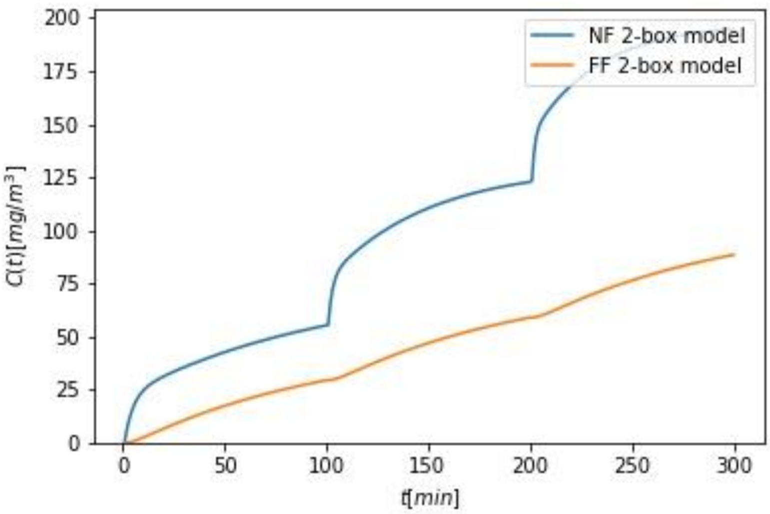

Figure 7: Output concentrations during case 4.

Case 5 is a variation of Case 1 with another type of ventilation in the room in which a LEV is applied, with an efficiency of capture of 75%.

TABLE 10: INPUT PARAMETERS CASE 5		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	1	
Ventilation type	v3	general ventilation + LEV
beta	3	m^3/min
Q	20	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 11: MODEL OUTPUT CASE 5				
	Near Field		Far Field	
Steady State mass concentrations:	2,80	mg/m^3	0,30	mg/m^3
Average mass concentrations for the whole cycle:	2,729	mg/m^3	0,276	mg/m^3
Average particle concentrations for the whole cycle:	4,170e+10	#/cm^3	4,217e+09	#/cm^3
8-hour concentration	2,001e+13	#/cm^3	2,024e+12	#/cm^3

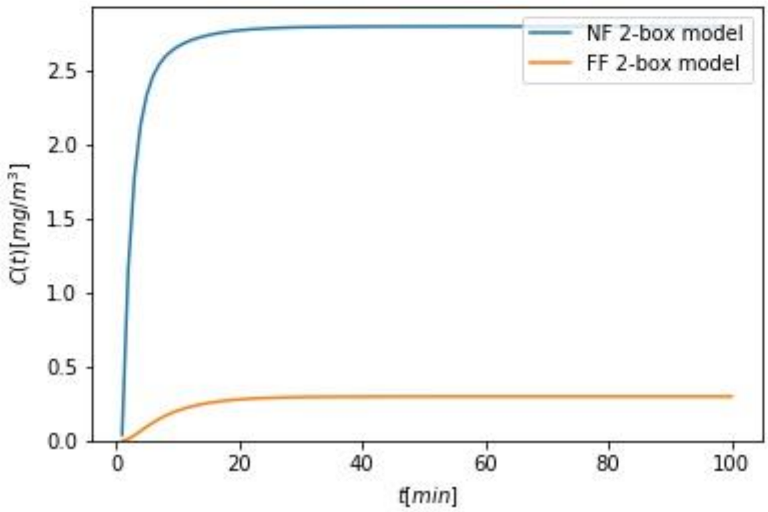

Figure 8: Output concentrations during case 5.

In comparison with case 1, it can be seen in Figure 8 how in first place the steady state is reached in matter of minutes and how the concentrations are reduced, especially in the Far Field.

Case 6 is a variation of Case 5 with 3 repetitions of the action with no pause in between. As in case 4, it can be seen in Figure 9 how the concentration increases progressively for each repetition, although the steady state concentrations reach the same values as in case 5.

TABLE 12: INPUT PARAMETERS CASE 6		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	3	
Ventilation type	v3	general ventilation + LEV
beta	3	m^3/min
Q	20	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 13: MODEL OUTPUT CASE 6				
	Near Field		Far Field	
Steady State mass concentrations:	2,80	mg/m^3	0,30	mg/m^3
Average mass concentrations for the whole cycle:	5,546	mg/m^3	0,575	mg/m^3
Average particle concentrations for the whole cycle:	8,474e+10	#/cm^3	8,788e+09	#/cm^3
8-hour concentration	4,068e+13	#/cm^3	4,218e+12	#/cm^3

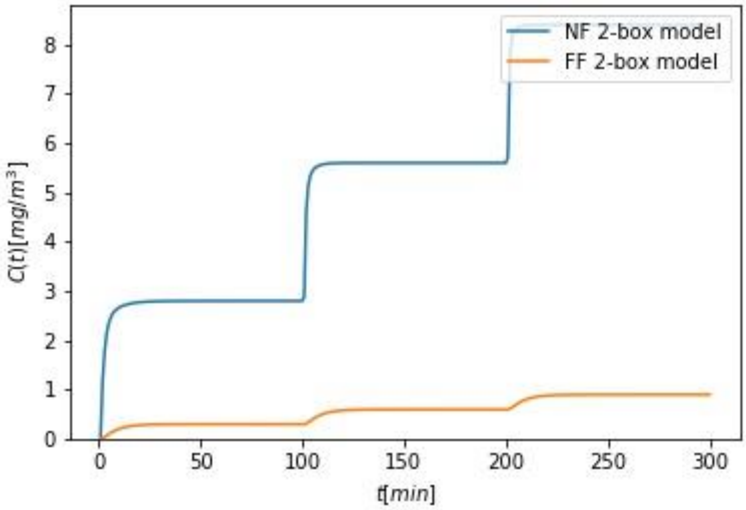

Figure 9: Output concentrations during case 6.

Case 7 is a variation of Case 1 with different type of ventilation, in which, besides of a LEV with air filtration efficiency of 99,9%, there is recirculation and filtration of the general ventilation in the room with an efficiency of 90%.

TABLE 14: INPUT PARAMETERS CASE 7		
Mass	100	g
Volume of facility	100	m^3
Activity duration	60	min
Pause between activities	0	min
Number of repetitions	1	
Ventilation type	v6	general ventilation + recirculation & filtration + LEV recirculation
beta	3	m^3/min
Q	20	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 15: MODEL OUTPUT CASE 7				
	Near Field		Far Field	
Steady State mass concentrations:	2,72	mg/m^3	0,22	mg/m^3
Average mass concentrations for the whole cycle:	2,658	mg/m^3	0,204	mg/m^3
Average particle concentrations for the whole cycle:	4,061e+10	$\#/cm^3$	3,113e+09	$\#/cm^3$
8-hour concentration	1,949e+13	$\#/cm^3$	1,494e+12	$\#/cm^3$

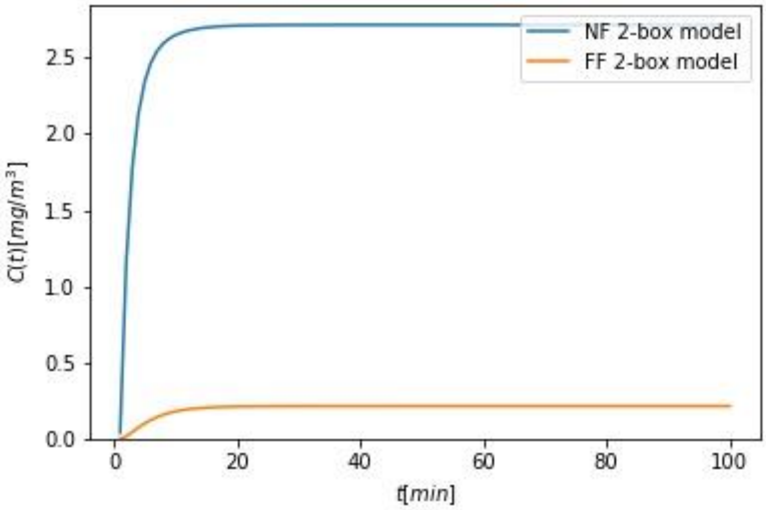

Figure 10: Output concentrations during case 7.

In Figure 10 it can be seen although the plot is very similar to case 5, concentrations, especially in the far Field, are slightly reduced.

Case 8 is a variation of Case 7 but with 20 minutes of pause within the 1-hour duration. This causes a decay of the concentrations to the background level if no other source is contributing, as can be seen in Figure 11.

TABLE 16: INPUT PARAMETERS CASE 8		
Mass	100	g
Volume of facility	100	m^3
Activity duration	40	min
Pause between activities	20	min
Number of repetitions	1	
Ventilation type	v6	general ventilation + recirculation & filtration + LEV recirculation
beta	3	m^3/min
Q	20	m^3/min
Mt	100	mg/min
Er0	80	mg/min
Background concentration	0	mg/m^3

TABLE 17: MODEL OUTPUT CASE 8				
	Near Field		Far Field	
Steady State mass concentrations:	4,07	mg/m^3	0,32	mg/m^3
Average mass concentrations for the whole cycle:	2,717	mg/m^3	0,215	mg/m^3
Average particle concentrations for the whole cycle:	4,151e+10	#/cm^3	3,291e+09	#/cm^3
8-hour concentration	1,992e+13	#/cm^3	1,580e+12	#/cm^3

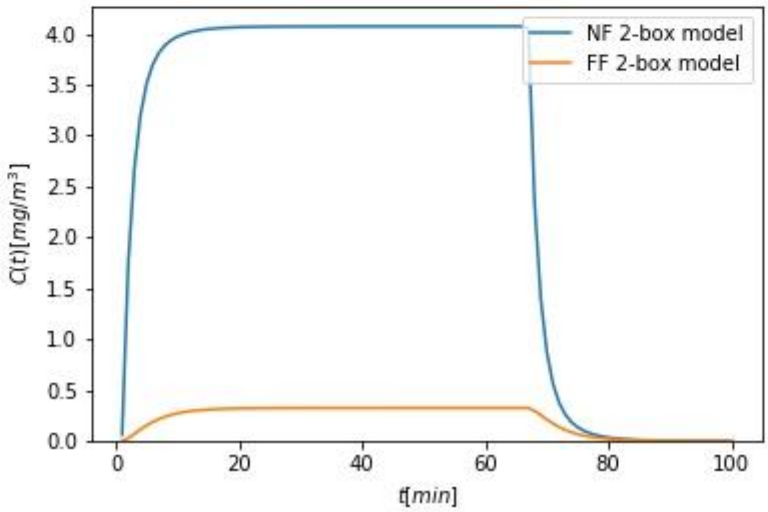

Figure 11: Output concentrations during case 8.

All these cases evidence the amount of possibilities of the model, which shall be tested against real cases with measurements in controlled situations to prove their accuracy.

3.2. Preliminary definition of the web tool lay-out

The model is divided in 3 main parts (figure 12):

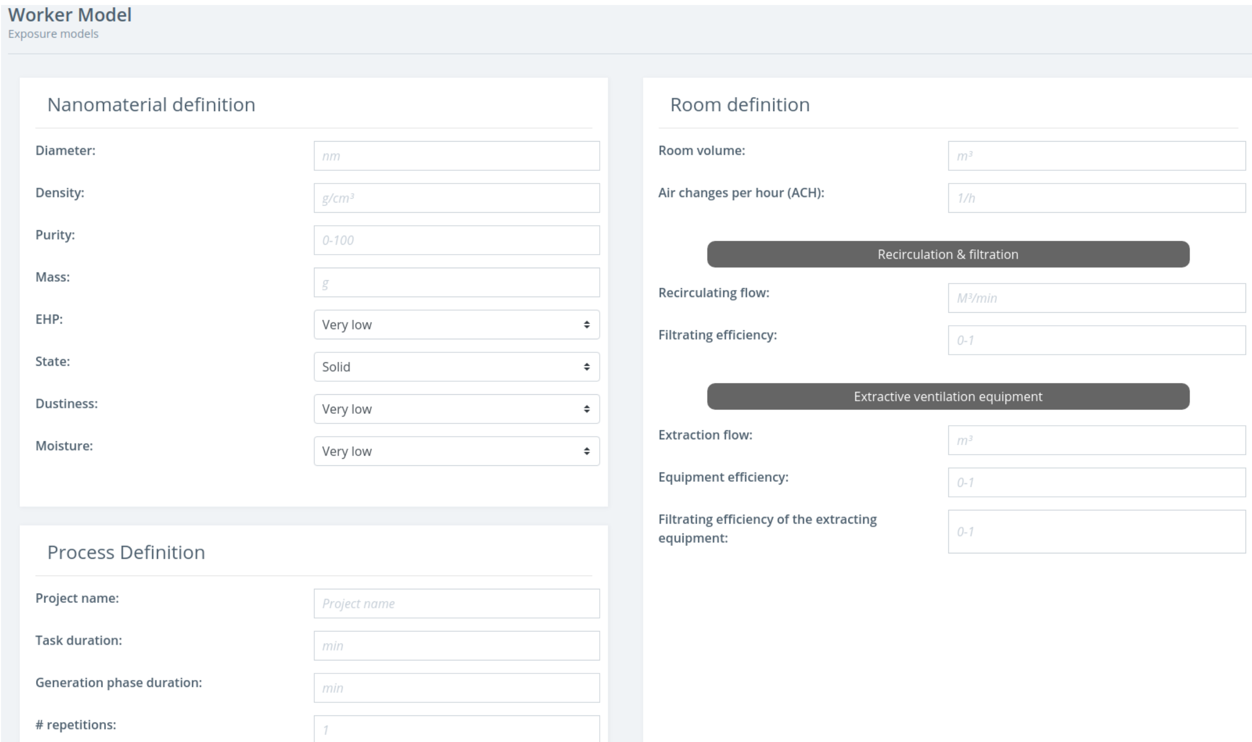

Figure 12: General view of the model: total mass handled, name given by the user and commercial and other relevant parameters.

- **Definition of the nanomaterial**: The code needs to be provided with different characteristics of the NM, in order to perform the calculation properly (figure 13).

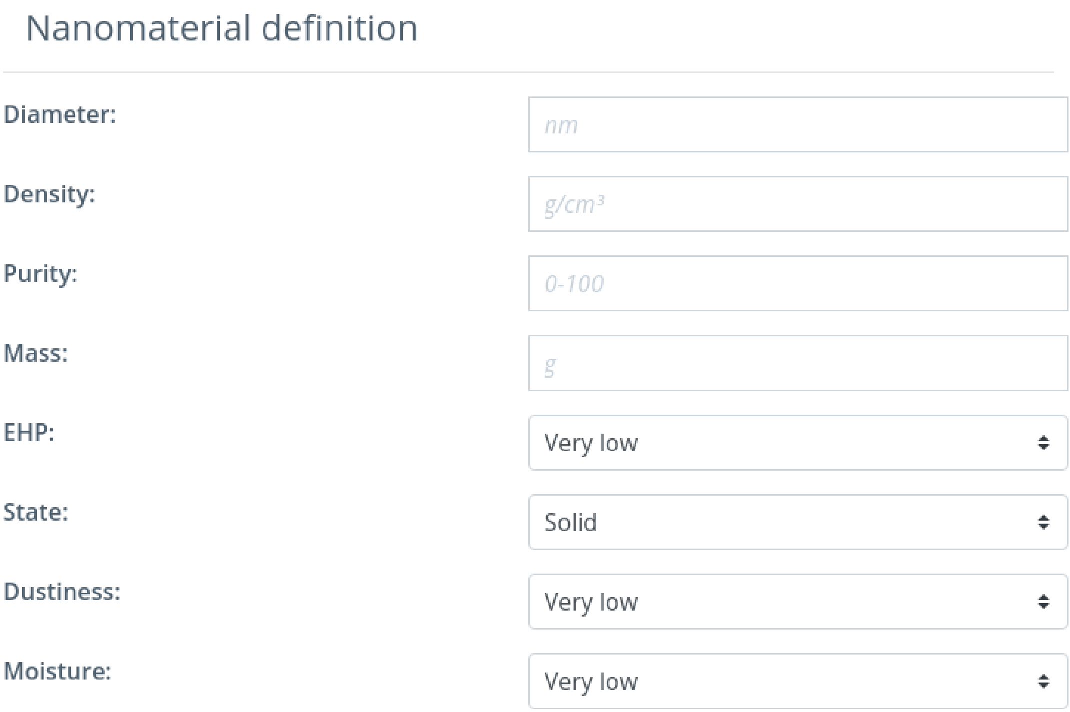

Figure 13: Nanomaterial definition: a detailed description of the ENM can be introduced.

- **Definition of the process**: The calculations running in the backend will lead to a solution of the differential equations: the near field and far field concentrations C_{NF} and C_{FF} as a function of the time. These equations also take into account the details of how and for how long the NM is released into the environment (figure 14).

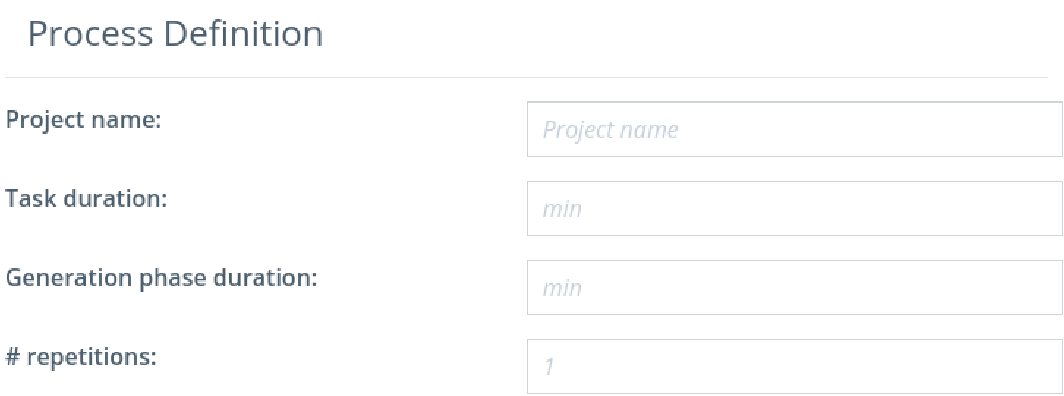

Figure 14: Process definition: duration of the activities (including pauses and repetitions) can be inserted.

- **Definition of the scenario (room):** where the user defines the room where the release of the NMs is taking place. Many options are given depending on the extractive system that is installed (figure 15).

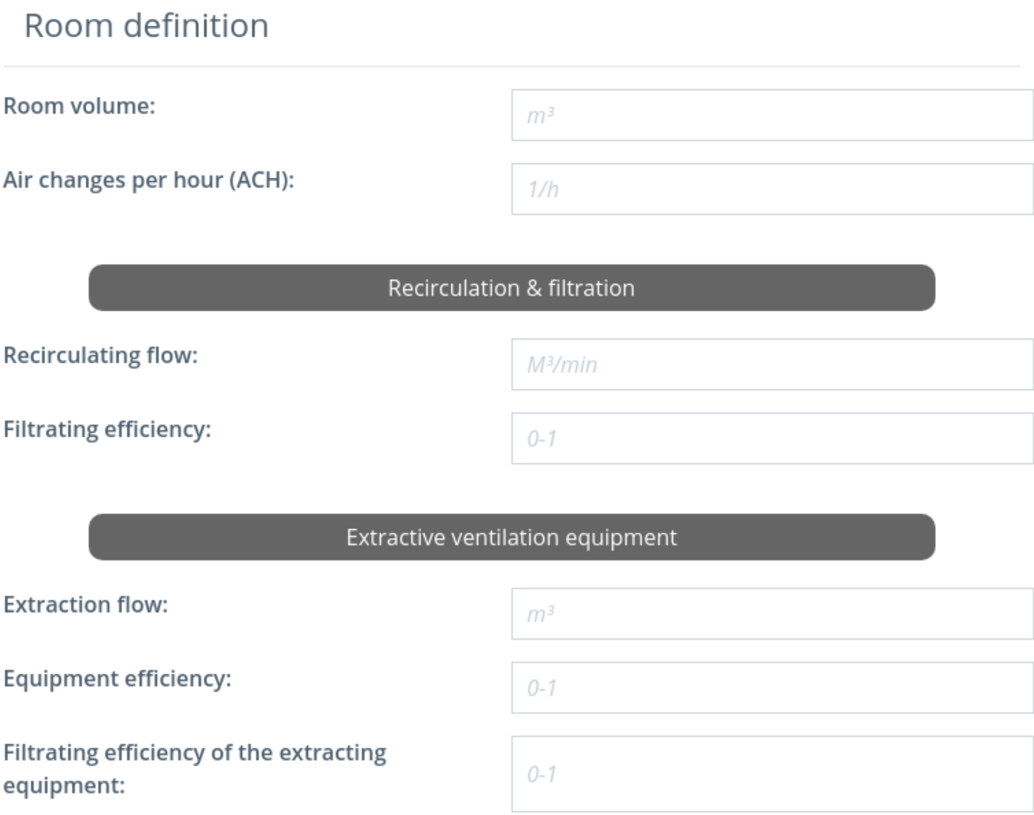

Figure 15: Room definition.

4. Discussion

The goal of the task 4 of the NanoDESK project is to propose several models which can quantitatively predict the fate and transport of the airborne ENMs released from processes related to the plastic sector in workplaces and in the environment. For this purpose, several current models were revised to establish a base of the processes and properties of the ENMs which can predict their influence and relevance on the risk of emission.

The Occupational model presented in this document was mathematically developed as a set of mass balance ODEs (Ordinary Differential Equations) and coded in Python. Transformation between mass and particle number concentrations is included.

Several performance tests were completed to analyze the scope of the model and a pre-design of the layout to be implemented in the tool repository of the NanoDESK platform was drafted.

Next steps are to complete the definitive design of the model interface and upload it for user-testing in the platform and compare the predicted results from the model with real measurements, to perform an accuracy and consistency test.

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