# GUIDEnano

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# Example of Use in "Pouring small bags of TiO2 powder" case study

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| Version log *[Add lines if needed]* | | | |
|---|---|---|---|
| **Version** | **Date** | **Author** | **Change** |
| 1.0 | | | First draft |
| | | | First revision |
| | | | Second revision |
| | | | |
| | | | Final version |

| *Keywords [up 5 keywords should be sufficient]* |
|---|
| GUIDEnano, Case study example, Pouring of TiO2 RD3 |

# Table of Content



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# 1 Tool description and use domain(s)

*[Guidance: Please give a brief description of the tool and its application domain(s)]*

GUIDEnano is a risk assessment model that allows the assessment and mitigation of human and environmental risks related to nanomaterials (NM) and nano-enabled product (NEP), considering their whole life cycle. Using GUIDEnano Tool, different stakeholders can evaluate and efficiently mitigate possible health risks for workers, consumers and the environment.

GUIDEnano is currently still under development and the aim of its future versions is to improve the user friendliness of the model by including more default parameters by connecting databases for the (nano)material characterizations and by adding libraries to provide process/activity related information/data.

# 2 Description of case study

*[Guidance: This section explains the technical material and/or experimental methods used and / or applied in the deliverable. Please use graphics as appropriate.]*

To run an example Case study in GUIDEnano it was decided to use one high-quality data literature paper from Koivisto et al. "Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory", Environ. Sci.: Processes Impacts, 2015,17, 62-73. In specific, the example Case study explained below focus on one of the exposure scenarios (ES) described: the pouring of small bags (SB) of $TiO_2$ RD3, (Pouring process SB RD3) performed by the workers in a paint factory.

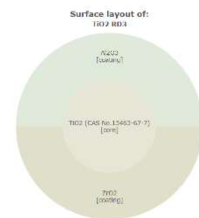
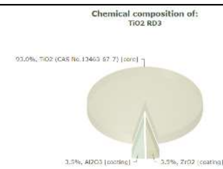
# 3 Input parameters

*[Guidance: Give the input parameters in table format (choose the type below that suits the data best)]*

Most of the input parameters needed to model this Case study, including the work environment, the process information and the NM characteristics, are provided from the literature paper. The table below report the input parameters required by GUIDEnano, indicating which data entry are recommended (R) or mandatory (M) and contains comment on the assumptions applied. The table below includes also some of the values and output provided by the Tool (written in gray color).

Table 1 Input parameters used for running a Case study in GUIDEnano

| N° | Entry Parameters | Input value | Comments, assumption and indication: R = Recommended parameter and M = Mandatory parameter |
|---|---|---|---|
| **GUIDEnano case** | | | |
| Identity | | | |
| 1 | Name of this case: | TiO2 case study (Koivisto 2015a_ Pouring 10 times 25 kg of TiO2 RD3) | R |
| 2 | General description and goal: | Koivisto AJ, Jensen ACØ, Levin M, et al (2015) Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory. Environ Sci Process Impacts 17:62–73. doi: 10.1039/C4EM00532EScenario | R |
| **(Nano)materials** | | | |
| Scenario relevant (nano)materials | | | |
| 3 | Select scenario relevant (nano)materials: | Nano-object | M |
| 4 | Name: | TiO2 RD3 | M |
| 5 | Description: | Nanomaterials used in the study | M |
| **Physico-chemical characteristic** | | | |
| Identification | | | |
| **6** | Name: | TiO2 RD3 | R |
| **7** | Description: | Nanomaterials used in the study (characterization provided in Table 1). Sachtleben Pigment GmbH, Pori, Finland, CAS 13463-67-7. Others provided: bulk density, d50, OEL, dustiness. Crystalline phase: rutile. Size: 220 nm, Normal distribution (assumption), 10% Standard deviation (assumption). | R |
| **8** | Origin: | Engineered | R |
| **9** | Source/supplier: | Sachtleben Pigment GmbH, Pori, Finland, CAS 13463-67-7 | R |
| Shape and size | | | |
| **10** | Shape | Spherical (assumption) | M, the shape of the particles is not reported (**assumption**). |
| **11** | Size distribution data available? | Yes | M |
| **12** | Method used: | Other | R. Analytical method to provide the size is not specified. |
| **13** | Size type: | Primary size | R |
| **14** | Metric of size distribution: | Mass | R |
| **15** | Distribution: | Normal | Normal distribution (**assumption**). |

| | | | |
|---|---|---|---|
| **16** | Mean size in nm: | 220 | |
| **17** | Standard deviation: | 22 | Standard deviation 22 nm (**assumption, 10% of main size**). |
| Physical properties | | | |
| **18** | Physical state of this material: | Solid | R |
| **19** | Indicate the size categorie(s) this solid material may present itself: | Ultrafine powder (100 nm-1µm); nanoscale particles (1nm-100 nm) | Automatically provided by the Tool according to the size provided. |
| **20** | Rigidity: | Rigid | R |
| **21** | Dustiness [mg/kg]: | 5.3 | R |
| Surface properties | | | |
| **22** | Layout and charge: | Chemical compound: TiO3 RD3, Role: core, contact order: 1. Chemical compound: Al2O3, Role: coating, Contact order: 2. Chemical compound: ZrO2, Role: coating, Contact order: 2. | R   |
| Other properties | | | |
| **23** | Functions | Pigment, UV filters | R |
| **24** | Chemical info | Are all constituents, impurities and contaminants added and identified? Yes. Purity in % :100 | R   |
| **Constituents** | | | |
| **25** | Mass density: | 4 g/cm3 | M |
| **26** | Select constituents | Category: chemical, name/identifier: TiO2 RD3 (CAS No.13463-67-7), phase: solid, role of constituent: core, conc.: 93, unit: %, mass perc.: 93% | M |
| **27** | Select constituents | Category: chemical, name/identifier: Al2O3, phase: solid, role of constituent: coating, conc.: 3.5, unit: %, mass perc.: 3.5% | M. **Assumption:** 3.5% is Al2O3 and 3.5 is ZrO2. |
| **28** | Select constituents | Category: chemical, name/identifier: ZrO2, phase: solid,role of constituent: coating,conc.: 3.5 ,unit: %,mass perc.: 3.5%. | M. **Assumption**: 3.5% is Al2O3 and 3.5 is ZrO2. |
| **Core: TiO2 RD3 (CAS No.13463-67-7)** | | | |
| Identification | | | |
| **29** | Chemically identified by: | Molecular formula. | M |
| **30** | Chemical name: | TiO2 (CAS No.13463-67-7) | R |
| **31** | Molecular formula: | TiO2 | M |

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| | | | |
|---|---|---|---|
| 32 | Avarage formula mass in [g/mol]: | 79.8658 | Automatically calculated. |
| 33 | Density: | 4.0 g/cm3 | M. From MSDS. |
| Physical properties | | | |
| 34 | Phase: | Solid | R |
| 35 | Rigidity: | Rigid | R |
| **Coating: Al2O3** | | | |
| Identification | | | |
| 36 | Chemically identified by: | Molecular formula. | M |
| 37 | Chemical name: | Al2O3 | R |
| 38 | Molecular formula: | Al2O3 | M |
| 39 | Avarage formula mass in [g/mol]: | 101.9612 | Automatically calculated. |
| Physical properties | | | |
| 40 | Phase: | Solid | R |
| 41 | Rigidity: | Rigid | R |
| **Coating: ZrO2** | | | |
| Identification | | | |
| 42 | Chemically identified by: | Molecular formula. | M |
| 43 | Chemical name: | ZrO2 | R |
| 44 | Molecular formula: | ZrO2 | M |
| 45 | Avarage formula mass in [g/mol]: | 123.228 | Automatically calculated. |
| Physical properties | | | |
| 46 | Phase: | Solid | R |
| 47 | Rigidity: | Rigid | R |
| **Activities** | | | |
| 48 | Activity name: | Pouring 25 kg RD3. | R |
| 49 | Setting/scale: | Large industry. | R |
| 50 | Life cycle phase: | Production. | R |
| General info | | | |
| 51 | Activity name: | Pouring 25 kg RD3. | R |
| 52 | Setting/scale: | Large industry. | R |
| 53 | Handling type: | Manual. | R |
| 54 | Applied energy level: | Medium. | R |
| 55 | Life cycle phase: | Production. | R |
| 56 | Concurrent locations: | 1 | M |
| Input, Output and release | | | |
| 57 | Activity input: | Input description: total amount of TiO2 nanomaterial poured during the activity, Material: TiO2 RD3, Total amount: **250**, Unit: | M |

| | | | |
|---|---|---|---|
| | | **kg**, Ref.: yes, Rate: **25 kg/min**. | |
| 58 | Activity output(s): | Output description: TiO2 contained in the formulated paint, Material: TiO2 RD3, Relative to: Input/ TiO2 nanomaterial poured during the activity, Relative amount: **99.99947 %**, Total amount: **249.998675**, Unit: **kg**, Ref.: no. | M. Remaining % after the activity (total amount- total release). |
| 59 | Activity release(s): | Release description: Emitted particles into the room (indoor), Material: TiO2 RD3, Relative to: Input \| TiO2 nanomaterial poured during the activity, Relative release: **0.0005512 %**, RMM: yes with 90% of efficiency, Total release: 0,0001325, Unit: kg, Ref.: no, Rate/location: 13.25 mg/min. | M. Total mass released divided by total mass involved in the activity. Calculated using the NM dustiness. |
| Duration | | | |
| 60 | Activity repetition: | 1 | M |
| 61 | Operational time: | The operational time needed to complete this activity is 10 min based on the given rate and amount of material involved. There is an idle time 1 min after each pouring event. Activity is operational during: 24 h/day. | M |
| 62 | Time span: | Total time span of all activity cycles together: 20 min. | M |
| (Nano)material flow | | | |
| | Input: | Input: TiO2 nanomaterials that are poured during the activity. | OUTPUT, Automatically provided. |
| | Output(s): | Output(s): TiO2 contained in the formulated paint. | OUTPUT, Automatically provided. |
| | Release(s): | Release(s): Release \| Emitted particles into the room (indoor), Into compartment \| zone: Factory hall \| NF (LCLZ). | OUTPUT, Automatically provided. |
| Local controls | | | |
| 63 | Local controls | Yes, 90% efficiency | M |
| **Compartments** | | | |
| 64 | Select compartment: | Type: indoor air, Name: Factory hall. | M |
| 65 | Select compartment: | Type: outdoor air, Name: Outdoor air (outside of the factory hall). | M |
| **Factory hall** | | | |
| General | | | |
| **66** | Name: | Factory hall. | R |
| **67** | Width of the room | 20 m | M |
| **68** | Length of the room | 30 m | M |
| **69** | Height of the room | 2.5 m | M |
| **70** | Volume of the room | 1500 m3 | Automatically calculated. |
| Zones | | | |

| | | | |
|---|---|---|---|
| **71** | Select zone: | Zone description: **NF (LCLZ)**, Number: 1, Medium: air, Size: 8, Unit: m3, Total dimension: 8 m3. | M |
| **72** | Select zone: | Zone description: **Floor**, Number: 1, Medium: solid, Size: 600, Unit: m2, Total dimension: 600 m2. | M |
| **73** | Select zone: | Zone description: **Rest of the room (FF)**, Number: 1, Medium: air, Size: 1492, Unit: m3, Total dimension: 1492 m3. | M |
| **Zone: NF (LCLZ)** | | | |
| **74** | Properties: | Temperature: 25.0 ° C, Pressure: 1 atm. | R |
| **75** | Contact zones: | In contact with: **Floor**, Orientation: below, Separated: virtually.<br>In contact with: **Rest of the Room (FF)**, Orientation: around, Separated: virtually. | M |
| **76** | Exposed: | Select or add a new exposed human population or eco species: **Workers \| exposure NF (LCLZ)**. | M |
| **Zone: Floor** | | | |
| **77** | Properties: | Temperature: 25.0 ° C. | R |
| **78** | Contact zones: | In contact with: **NF (LCLZ)**, Orientation: above, Separated: virtually.<br>In contact with: **Rest of the Room (FF)**, Orientation: above, Separated: virtually. | M |
| **79** | Exposed: | Select or add a new exposed human population or eco species: Workers \| exposure Floor. | M |
| **Zone: Rest of the Room (FF)** | | | |
| **80** | Properties: | Temperature: 25.0 ° C, Pressure: 1 atm., Mechanical ventilation: Yes, Air exchanges per hour [/h]: 5. | M |
| **81** | Contact zones: | In contact with: **NF (LCLZ)**, Orientation: within, Separated: virtually.<br>In contact with: **Floor**, Orientation: below, Separated: virtually.<br>In contact with: **Outdoor air (outside of the factory hall) \| outdoor air**, Orientation: around, Separated: physically. | M |
| **82** | Exposed: | Select or add a new exposed human population or eco species: **Workers \| exposure Rest of the room (FF)**. | M |
| **Exposure \| Hazard assessment** | | | |
| **83** | Select human populations: | Population name: Workers, Group: Workers. | M |
| General | | | |
| **84** | Population name: | Workers. | R |

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| | | | |
|---|---|---|---|
| **85** | Population category: | Workers. | M |
| Exposure paths | | | |
| **86** | Select indirect through zones: | Exposure zone(s): **factory hall** \| **NF** (**LCLZ**), Route(s): inhalation, Exposure relevant material: TiO2 RD3. | M |
| **87** | Select indirect through zones: | Exposure zone(s): **factory hall** \| **Rest of the room** (**FF**), Route(s): inhalation, Exposure relevant material: TiO2 RD3. | M |
| 88 | Select indirect through zones: | Exposure zone(s): **factory hall** \| **Floor**, Route(s): dermal, Exposure relevant material: TiO2 RD3. | M |
| inhalation \| exposure NF (LCLZ) (TiO2 RD3) | | | |
| **89** | Concentration estimates: | Source/model: zone derived estimate, route: inhalation, peak estimate: 166,7 µg/m3, long term concentration: 51,2 µg/m3, Use: "v" (thick), PPE: not applied | M |
| **90** | Protective equipment used: | Not applied to this case because we want to model a "worst case scenarios" and make a risk assessment for workers in this situation. | M |
| **91** | Population presence: | Total timespan to consider: 1 year, During: 210 day(s)/year, Frequency: 1/day, Period of presence in zone: 10 minutes | M |
| inhalation \| exposure FF (TiO2 RD3) | | | |
| **92** | Concentration estimates: | Source/model: zone derived estimate, route: inhalation, peak estimate: 43,29 µg/m3, long term concentration: 0,71 µg/m3, Use: "v" (thick), PPE: not applied | M |
| **93** | Protective equipment used: | Not applied to this case because we want to model a "worst case scenarios" and make a risk assessment for workers in this situation. | M |
| **94** | Population presence: | Total timespan to consider: 1 year, During: 210 day(s)/year, Frequency: 1/day, Period of presence in zone: 10 minutes | M |
| Exposure scenarios | | | |
| | Exposure scenario | Exposure scenarios description: Pouring of 25 kg of TiO2 RD3 10 times with emission control, Exposure relevant material: TiO2 RD3 | OUTPUT, Automatically generated. |
| | Contributing path(s): | Pathway: exposure NF (LCLZ), Presence/contact: 10 minutes a day, used concentration estimates: (inhalation) peak estimate: 166,7 µg/m3, long term concentration: 51,2 µg/m3 | OUTPUT, Automatically generated. |
| | Contributing path(s): | Pathway: exposure FF, Presence/contact: 10 minutes a day, used concentration estimates: (inhalation) peak estimate: 43,29 µg/m3, long | OUTPUT, Automatically generated. |

| | | | |
|---|---|---|---|
| | | term concentration: 0,71 µg/m3 | |
| Hazard assessment | | | |
| 95 | Workers \| repeated dose toxicity (inhalation) Exposure relevant material: TiO2 RD3 | STEP 1: Are there regulatory binding or provisional OELs/DNELs for the exposure relevant material? (long term exposure) **Yes** | M |
| 96 | Workers \| repeated dose toxicity (inhalation) Exposure relevant material: TiO2 RD3 | Dose descriptors: **OEL**, critical dose: **6 mg/m3**, unit: mg/m3, duration: long term, exposure relevant material: TiO2 RD3, source/comment: Table 1 in the paper | M |
| **Risk assessment** | | | |
| | Human exposure: Worker, Exposure scenario: Pouring of 25 kg of TiO2 RD3 10 times with emission control, | Hazard endpoint to assess: Repeated dose toxicity – Inhalation. Risk characterization ratio (RCR): 0,0004934 | OUTPUT, Automatically provided. |

# 4 Results

This example shows the different parameters on “Case, Nanomaterial, Activity performed (mass balance), Compartment where activity take place and Exposure information” that are required to run a Case study in GUIDEnano.

Most of the data on the “exposure relevant Nanomaterial” ($TiO_2$ RD3) are provided in the literature paper or can be found in the material safety data sheet. The NM shape, size and density are the most important data for the following conversion from “mass” to “particles” metrics in the different estimates.

The “Activity” information such as the amount of NM used, the duration of the activity and the activity emission rate, are mandatory parameters and the assumption applied for these values strongly affect the modeled NM concentration in the zone derived estimate. In this Case study, all the parameters except the activity release rate are reported in the paper. The release rate is calculated from the dustiness of the NM which was also reported in the literature paper (Table 1).

The “Compartment” information, especially the room dimension and the ventilation rate are very important parameters for a correct simulation of the working environment modeled. These parameters are described in the literature paper. For the final hazard and risk assessment is important to indicate the presence of the exposed population in the different zones (such as near field and far field), because GUIDEnano Tool consider these values for the final risk assessment and for the calculation of the Risk Coeffient Ratio (RCR).

The outputs of GUIDEnano Tool for this Case study are the NM concentration in the zone derived estimates that can be compared with measurement data provided in the literature paper and the RCR that provide an indication on the risk level for the considered exposure and hazard endpoint.

The GUIDEnano zone derived estimate in NF is 166,7 µg/m3 and the value reported in the paper is 167.1 µg/m3, which correlate very well with the modelling results. This result confirm that the assumption and the value used are good representation of the situation modelled.

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# I. Annex I

## *I.1. Further explanation to run the Case study example in GUIDEnano*

GUIDEnano Case from the literature paper published on Environ. Sci. Process. Impacts 17:62–73. doi: 10.1039/C4EM00532EScenario "Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory", Koivisto AJ, Jensen ACØ, Levin M, et al (2015).

GUIDEnano model needs different class of parameter on: Case, Nanomaterial, Activity performed (mass balance), Compartment where activity take place and Exposure information. This case is built gathering data and information from the exposure scenarios related to the pouring of small bag (25 kg) of TiO2 RD3 reported in the paper "Koivisto AJ, Jensen ACØ, Levin M, et al (2015) Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory", focusing on the pouring of small bags (25 kg) of TiO2 RD3.

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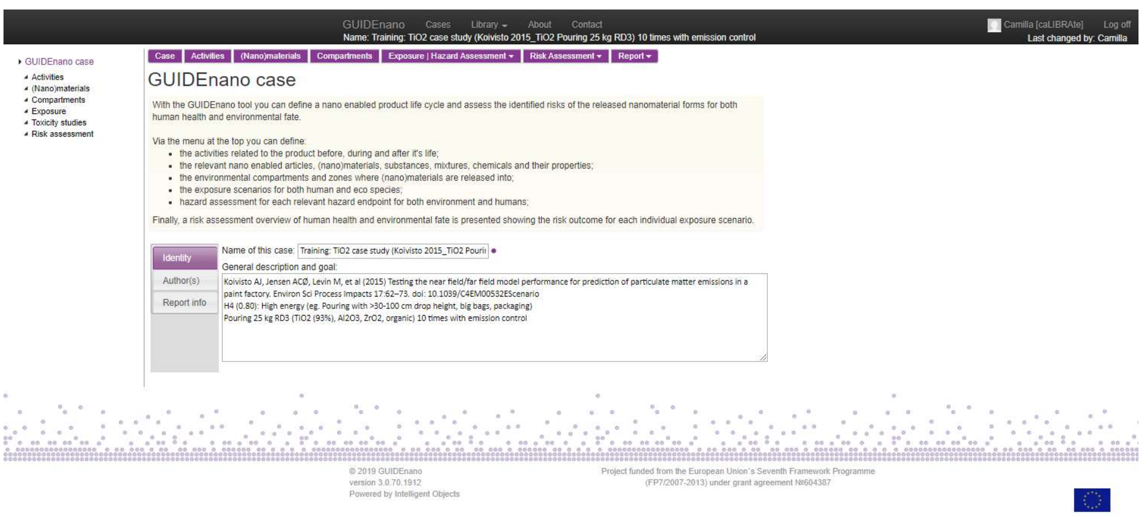
## GUIDEnano Case

To create a new Case, the user enters information on three tabs in the main page: Identity, Authors and Report info. The tab Identity can be filled with the name of the case (unique and identifying name) and its general description and goal. For the Case study example modelled, the name of the Case is “TiO2 case study (Koivisto 2015a_TiO2 Pouring 25 kg RD3)” and the general description and goal is “Koivisto AJ, Jensen ACØ, Levin M, et al (2015a) Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory. Environ Sci Process Impacts 17:62–73. doi: 10.1039/C4EM00532EScenario”, the specific ES modeled is the pouring of 25 kg bags of TiO2 RD3 for ten times with Local controls (SB RD3). The tab Authors and Report info can be filled with the corresponding information to provide more details on authors of the Case and on the kind of ES modelled.

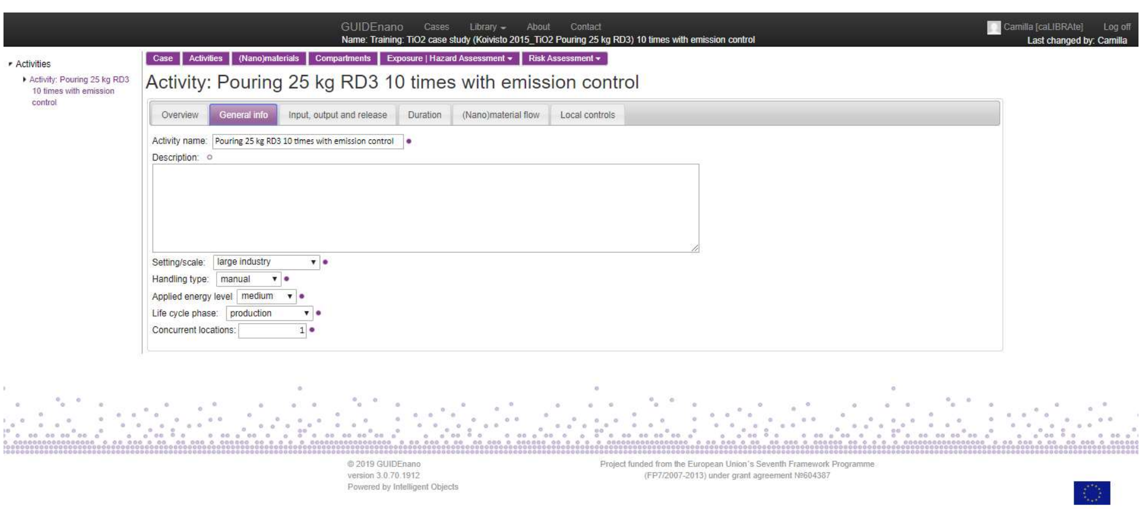


## Activities

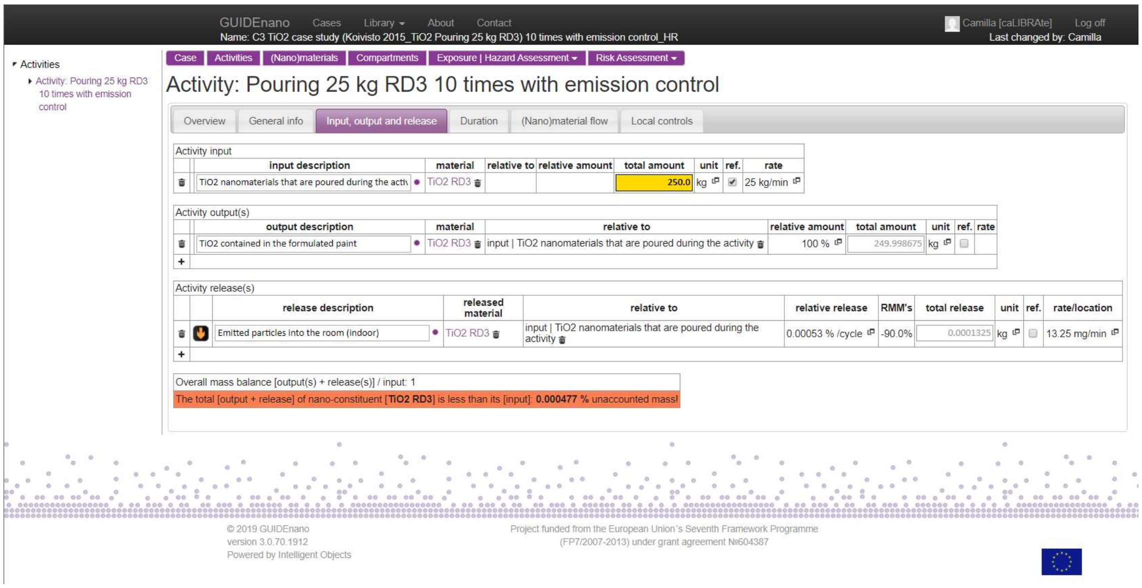
The activities framework allows a user to define all relevant activities within all stages of the life cycle of the nano-enabled product/article. Clicking on the "+", the user can define the activity, including information on activity name, setting/scale of activity, life cycle phase and number of concurrent location where activity take place.


In the case presented, only one activity is considered (in case that more than one activity is considered, the activities should be organized in the correct time order, starting with the earliest activity). To describe the activity, the user fills the following tabs: General info, Input, output and release, Duration and Local Control.

**General info**: requests an identifying name and a general description of the activity, the scale, the handling type, the applied energy level, the life cycle phase and the number of concurrent locations where the activity takes place.



**Input, output and release:** define the kind and the amounts of nanomaterial used within the activity using one input connector and multiple output and release connector(s), describing the activity through the mass balance of the involved NM.




The input connector defines the amount of nano(enabled) material the activity starts with (i.e.: for a pouring activity it would be the nanomaterials that will be poured in a bag/containers). The input connector must be filled with input description, material name, total amount, unit, reference (usually it is the reference nanomaterial for the mass balance of the activity), rate (i.e.: for a pouring activity it would be the amount of nanomaterial poured divided by the time of pouring this material). Output connectors are used to define the forms and amounts of material(s) leaving the activity but not entering any environmental compartment (i.e.: for a pouring activity it would be the nanomaterials poured in a bag/containers). The output connector must be filled with output description, material name, relative to (i.e.: for a pouring activity it would be relative to input), relative amount (it is the amount of output material relative to the input material), total amount, unit, reference and rate. Release connector are used to define the intended or incidental release amount/fractions of NM towards environmental compartments. A release connector is also used to enable direct contact exposure scenarios. The release connector has to be filled with release description, material name, relative to (i.e.: for a pouring activity it would be relative to input), relative amount (it is the amount of released material relative to the input material), risk mitigation measures (RMM's), total release, unit, reference, rate/location, describing the release rate per location. Internal mass flow: the connectors are also used to define the internal and the external mass flow between activities. In order to define the internal mass flow, the connectors need to be made relative to each other. In case an input and one or more output connectors are defined, the amount of at least one output connector is directly related to the input amount. A release may be made relative to either an input or an output connector.

In the Case modeled, the Activity Input is the $TiO_2$ nanomaterial ($TiO_2$ RD3) poured during the activity, the total amount is 250 kg with a (pouring) rate of 25 kg/min. The Activity output is the $TiO_2$ ($TiO_2$ RD3) contained in the formulated paint, the Relative amount (of input material) is the 99.99947%, corresponding to a total amount of 249.998675 kg. The Activity release is defined as the Emitted $TiO_2$ RD3 particles into the room (indoor), the Relative release is 0.0005512%, corresponding to a Total release of 0,0001325 kg. The Rate/location (transfer rate from the release source to the location where the release is ending up) is 13.25 mg/min. RMM is applied to the modeled situation, therefore to "simulate" the same condition reported in the paper a RMM with 90% of efficiency is included (by using the Local Control tab). The material output and the material release are made relative to the material input (which is the reference amount of material for this activity).

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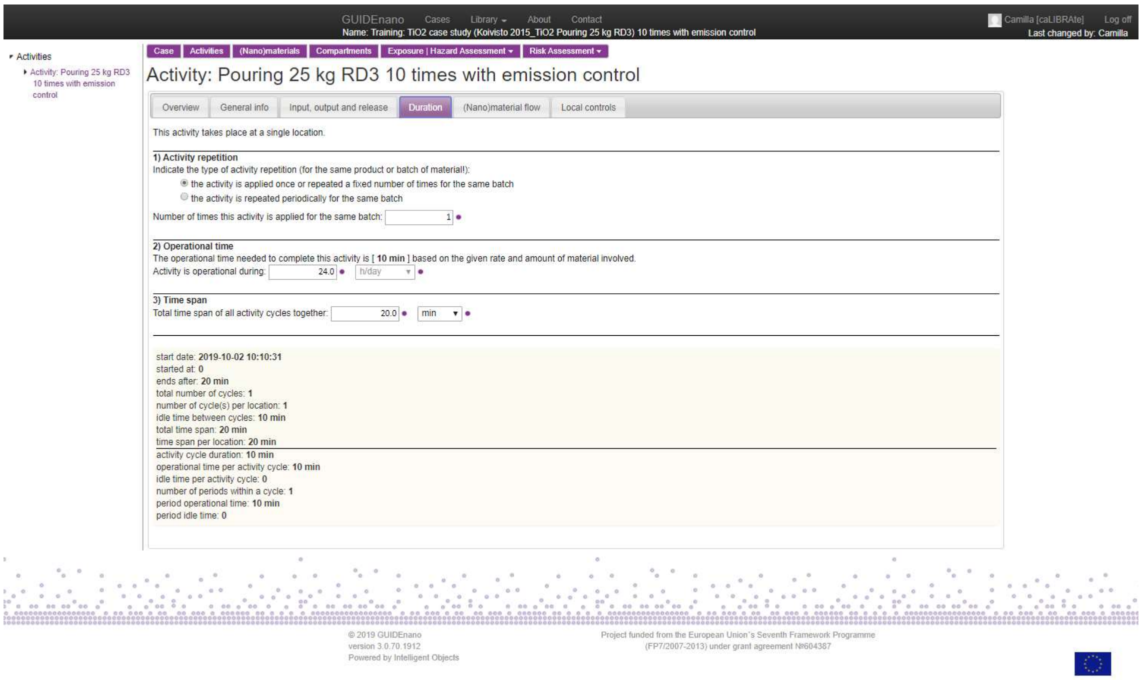
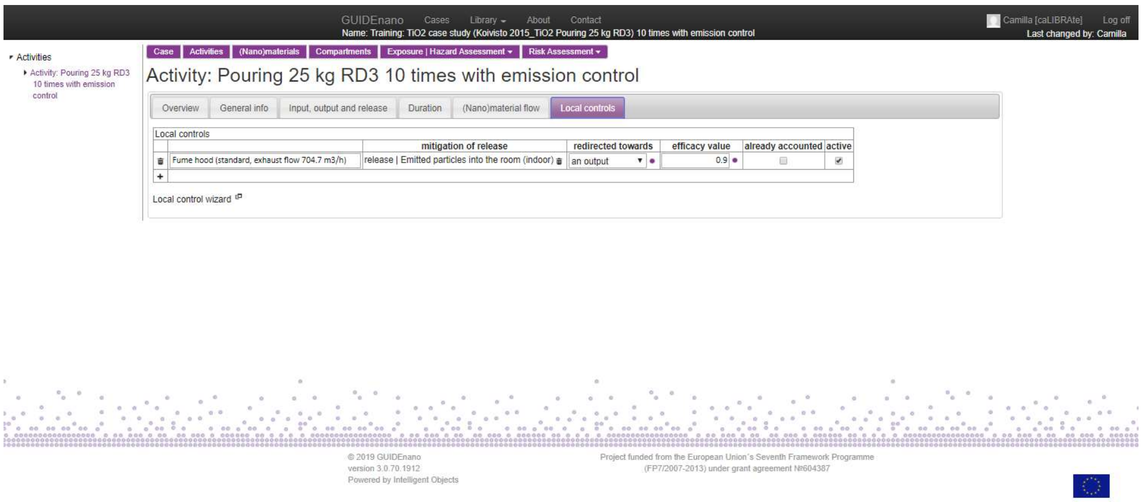
**Duration** tab: is used to define the time "properties" of an activity. In the entry Activity repetition, the user must indicate if an activity is repeated and if so, how many times (for the same batch!).

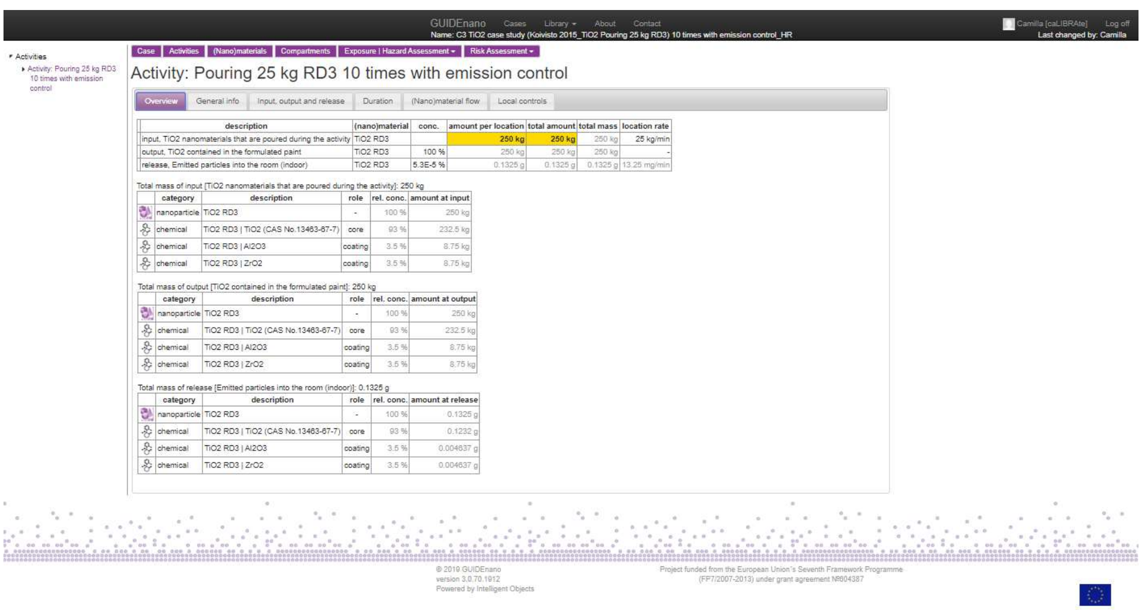


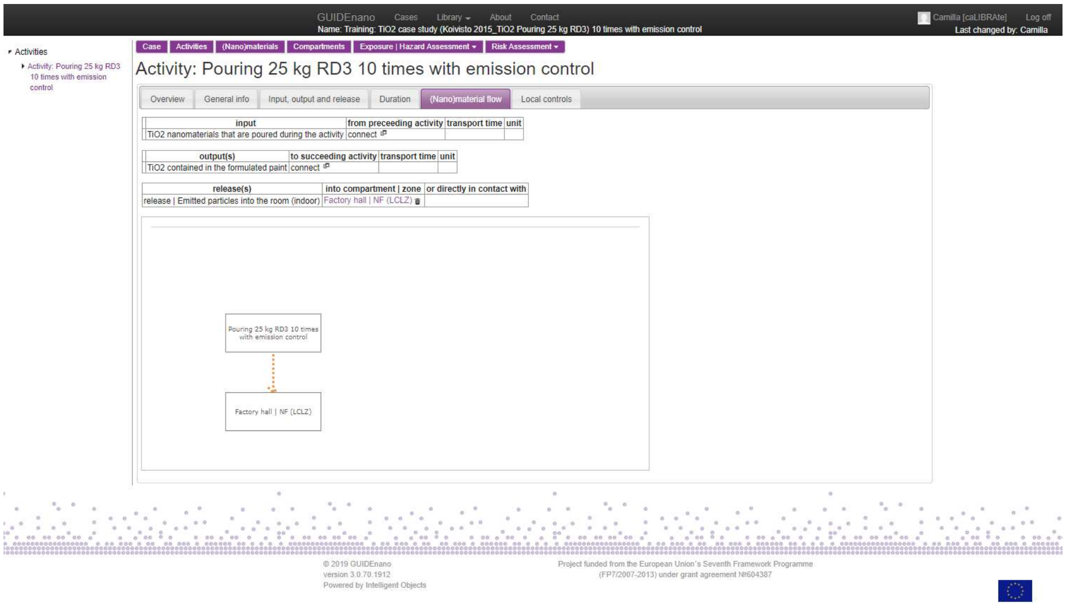

The operational time, or period, is the time needed to complete the activity based on the given (input or output) rate and (input or output) amount of material involved (i.e.: for a pouring activity the total amount of nanomaterial to be poured in kg and the rate of pouring in kg/min determines the total operational time in min needed). For this Case, the activity duration is defined with an operational time of 1 min and an idle time of 1 min, the activity is repeated 10 times, giving a total time span of 20 min. The operational time, determined by the input amount of nanomaterial to be poured in kg and the rate of pouring in kg/min, is 10 minutes.

**Local controls (release mitigation):** to mitigate a release is possible to apply local controls during the activity. In the ES selected, RMM were used, therefore an engineering controls with 90% of efficiency was applied.




The tabs **Overview** and **(Nano)material flow** information are automatically generated by the Tool once the previous tabs are filled by the user.




GUIDEnano Cases Library About Contact
Name: Training: TiO2 case study (Koivisto 2015_TiO2 Pouring 25 kg RD3) 10 times with emission control
Camilla [caLIBRAte] Log off
Last changed by: Camilla
Activities
Activity: Pouring 25 kg RD3 10 times with emission control
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input
from preceeding activity
transport time
unit
TiO2 nanomaterials that are poured during the activity
connect
output(s)
to succeeding activity
transport time
unit
TiO2 contained in the formulated paint
connect
release(s)
into compartment | zone
or directly in contact with
release | Emitted particles into the room (indoor)
Factory hall | NF (LCLZ)
Pouring 25 kg RD3 10 times with emission control
Factory hall | NF (LCLZ)
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version 3.0.70.1912
Powered by Intelligent Objects
Project funded from the European Union's Seventh Framework Programme
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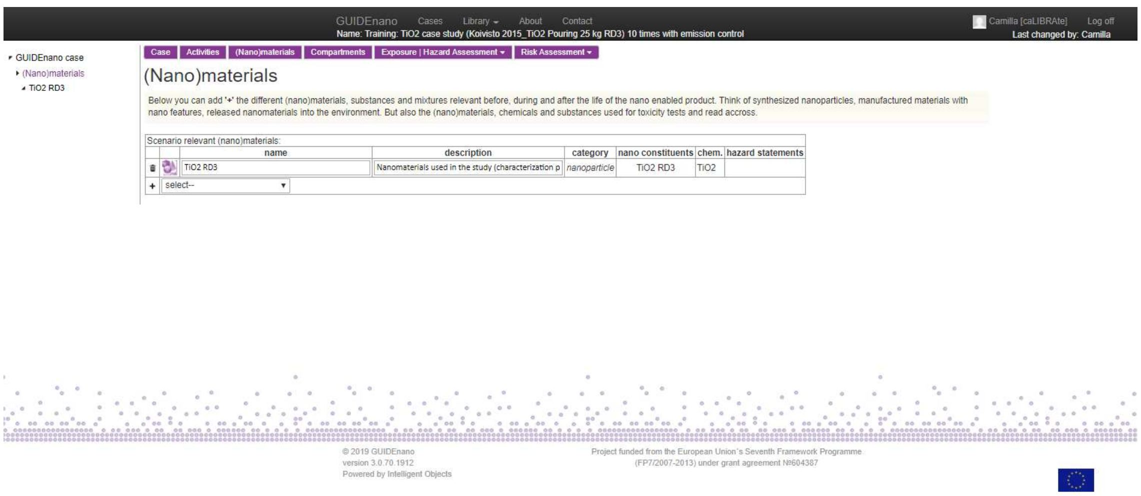
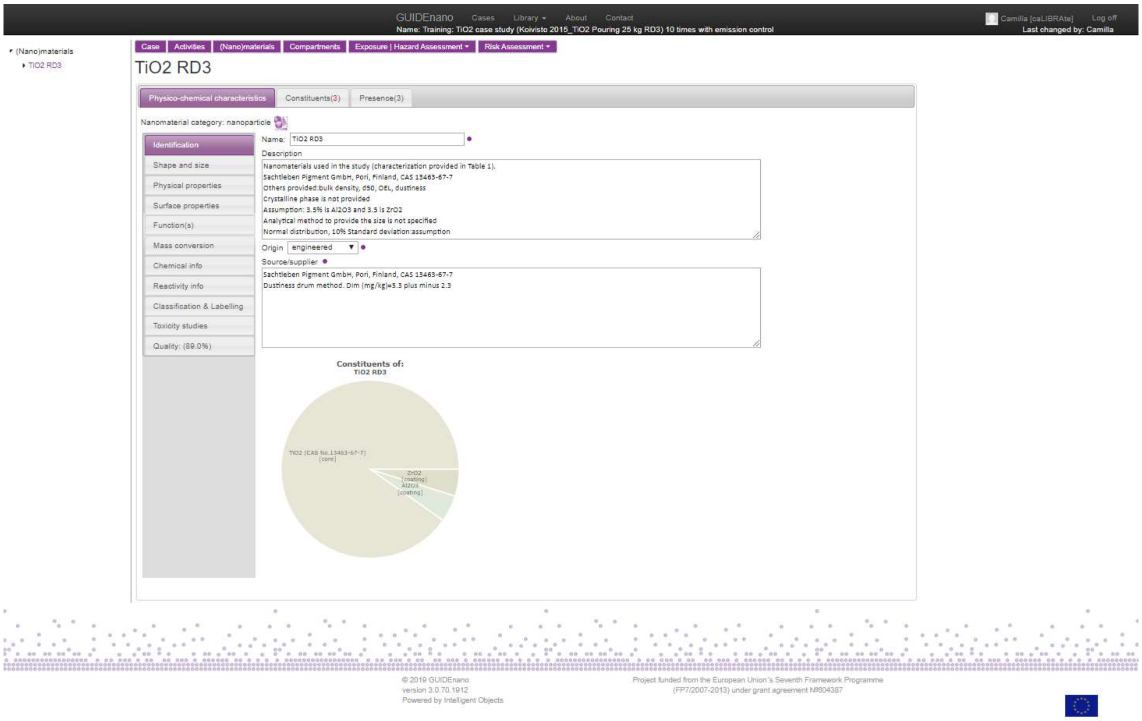
## (Nano)material framework

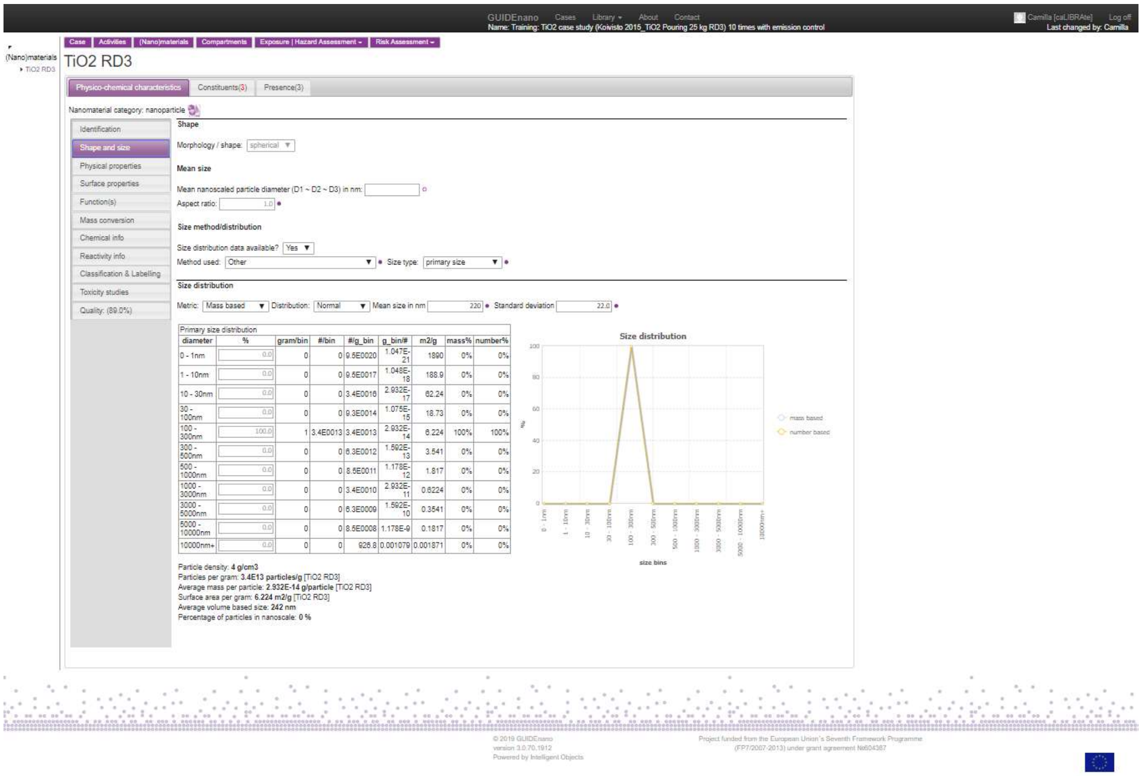
The (nano)material framework allows a user to define all life cycle relevant materials, substances, nanoobjects and nano-enabled products and articles. All defined materials need to be described including the under-laying components, chemicals and their role. To create a material, the user clicks "+" and selects the kind of material (article, substance/mixture, nano-object, nanostructured aggregate or nanostructured agglomerate), and add a short description. NOTE: in GUIDEnano a nanomaterial is currently considered to be either a NANO-OBJECT or a NANOSTRUCTURED MATERIAL as defined by the ISO/TS 80004-1:2010.



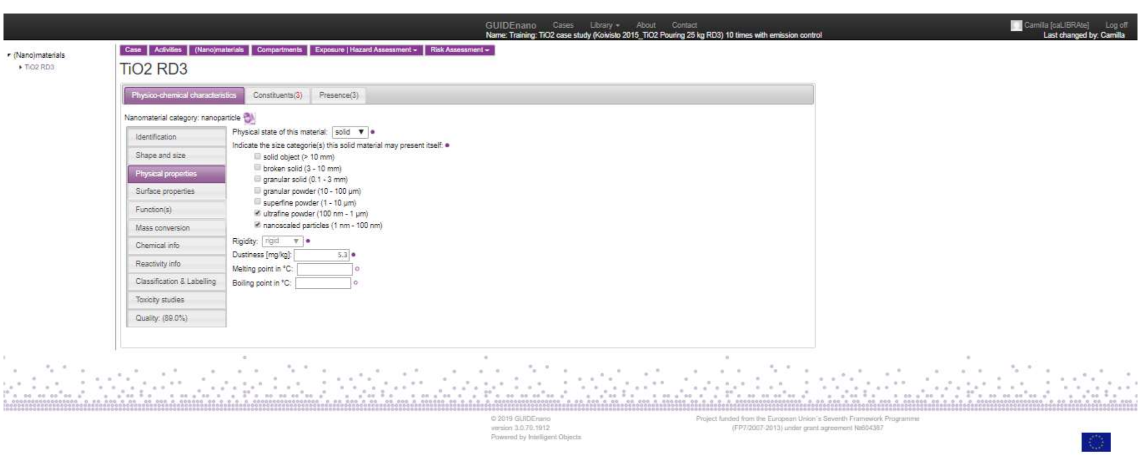

Once a new (nano)material has been created, the user can identify and characterize each material involved by filling the following tabs: Physico-chemical characteristics, Constituents and Presence. The **Physico-chemical characteristics** are described by the following tabs. **Identification:** The user enters a name for the material and can add a description and the source or origin of the material.



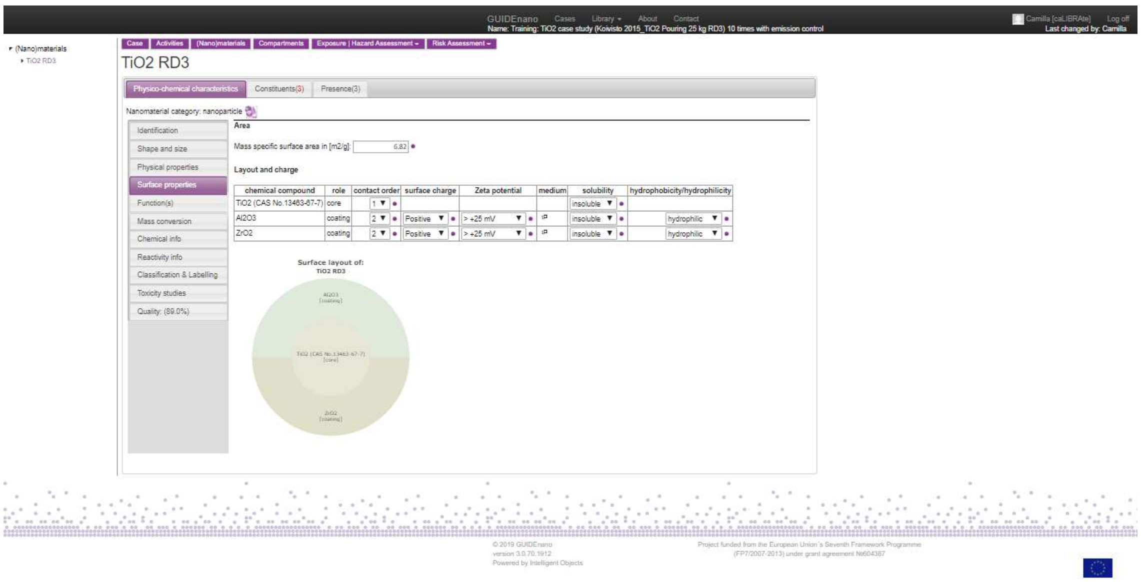

**Size and shape:** the user enter first the morphology of the nano-object (default spherical, cubes, wires, rods, tubes, platelets and discs). The selected shape determines the number of relevant external dimensions to enter. If a size distribution is available, the user can select which method was used and which size provides. Finally, the user can enter a primary size distribution for the nano-object. The distribution is described as a mass or number percentage of the nano-object per size bin (size bins used are: 0-1nm, 1-10nm, 10-30nm, 30-100nm, 100-300nm, 300-500nm, 500-1000nm, 10003000nm, 3000-5000nm, 5000-10000nm, 10000nm+). The user can either enter a value per bin or use a Log Normal or Standard Deviation. In this case a size of 220 nm is reported, and we assume to have a normal distribution with a 10% of standard deviation. Based on the size distribution, shape and density of the nano-object the tool can convert masses into particle numbers and vice versa.



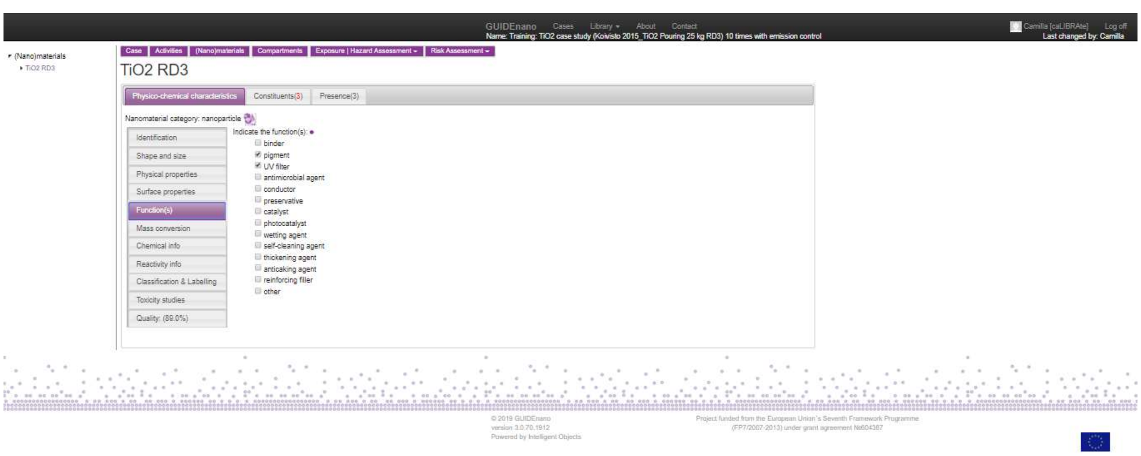

**Physical properties:** The user enters Physical state (ions, solid, liquid, gas and mixture). Depending on the state, different properties are requested, for example for a solid material, the Solid related properties includes Size categories, Rigidity, Dustiness (mg/kg), melting point and boiling point.



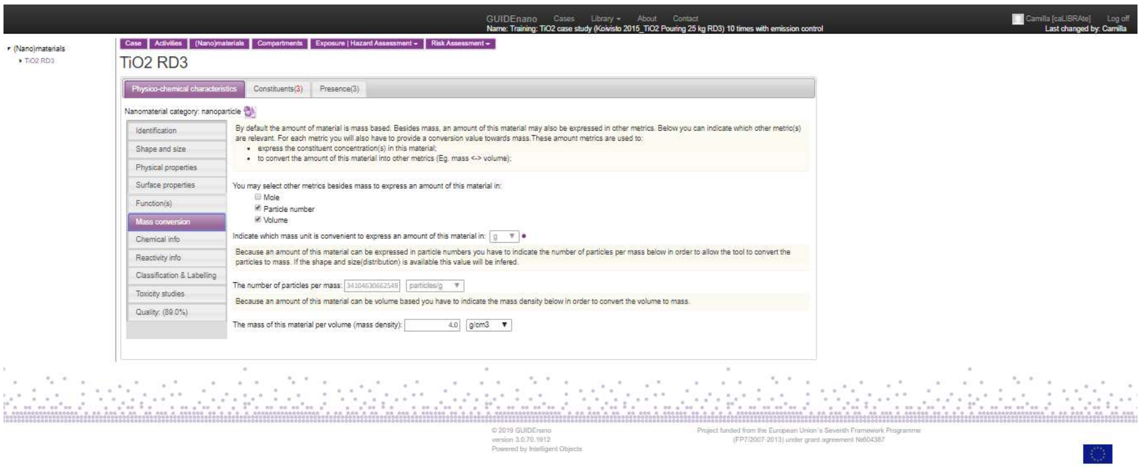
**Surface properties:** The user need to enter the mass specific surface area in m2/g and describe the Layout and charge for each constituent of the materials. The order of constituents is defined by an index. A higher index indicates a more outward layer and earlier external contact. Constituents may have the same index, indicating that they are part of the surface at the same time. Finally, information about the Surface charge, Zeta potential, Solubility and Hydrophobicity can be entered for each of the constituents placed in the most outward surface layer.



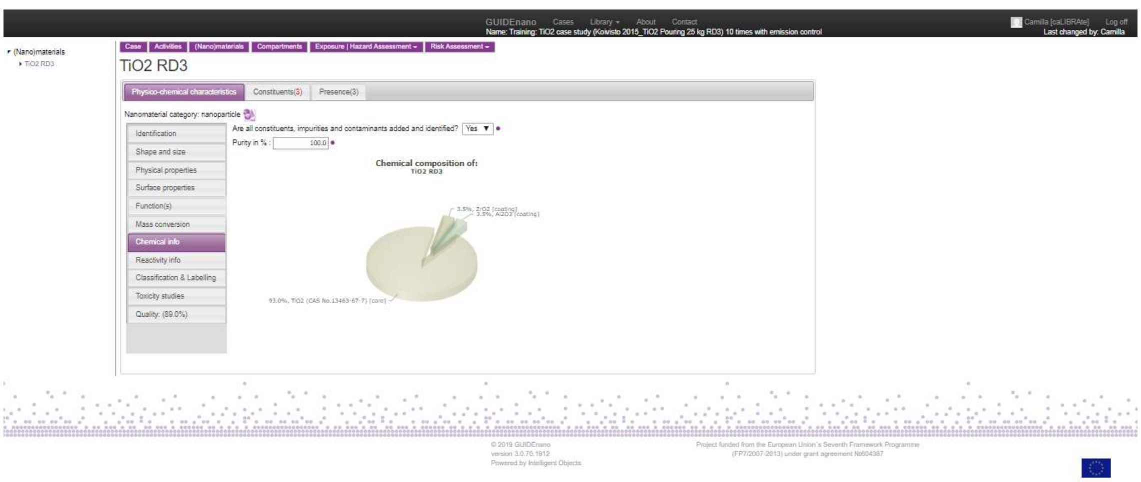

**Functions:** The user can add information about the "functional properties" of the (nano)material (pigment, UV filter, photo catalyst, etc.).



**Mass conversion:** The user can select different mass conversion metrics (mole, particle number, volume, surface area, …).



**Chemical info:** The users need to enter the material purity.



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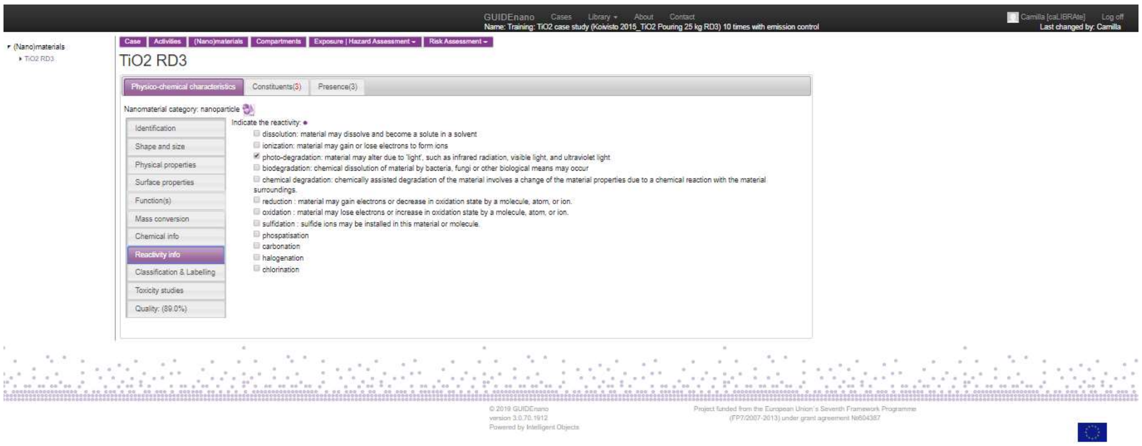
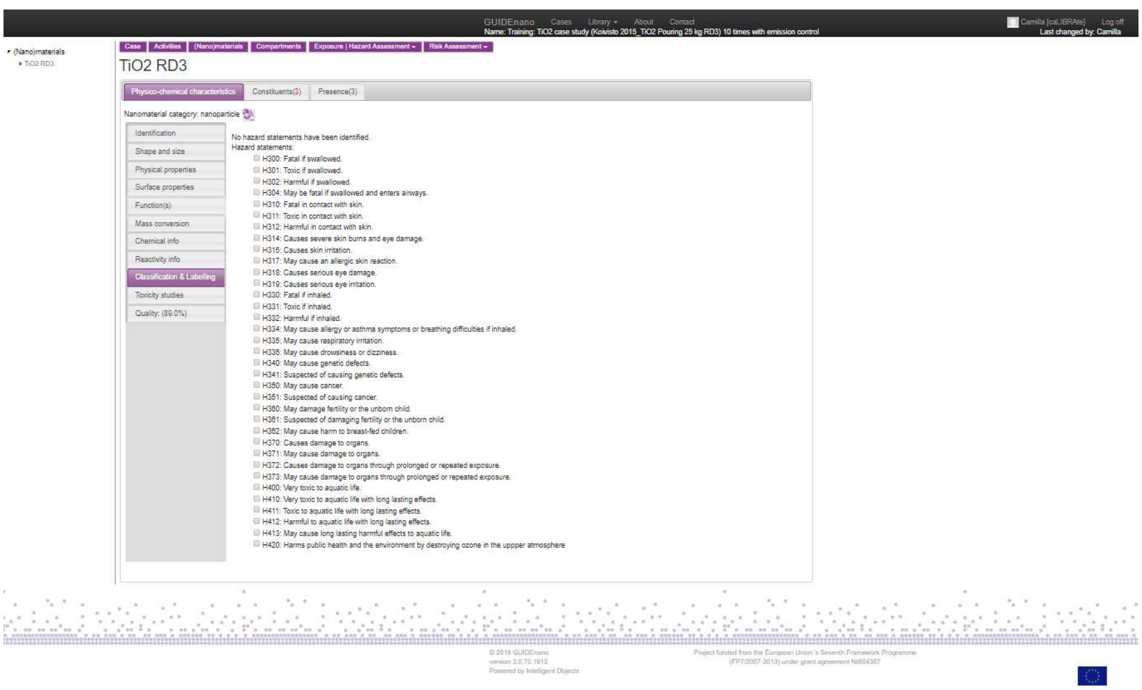
**Reactivity info:** The user can indicate multiple types of reactivity (dissolution, ionization, photo-degradation, …).




**Classification & Labelling:** The user can indicate if the material is labeled with any hazard statements according to the Global Harmonized System (GHS).

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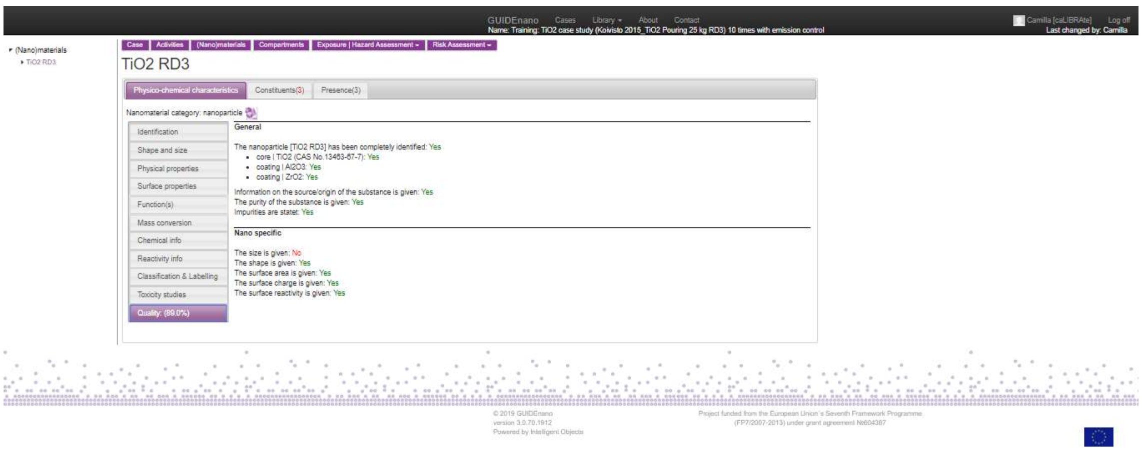
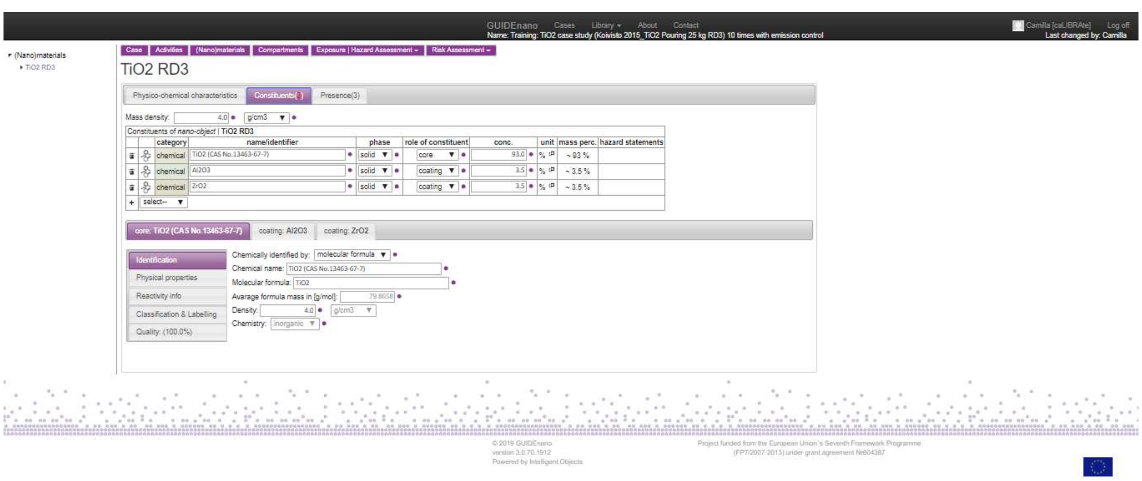
**Quality:** for the Hazard assessment, if toxicity data on relevant NM and endpoint (such as DNEL or OEL for inhalation exposure) are not available, the user can add Toxicity study related to the relevant NM or related to a similar NM. The Quality score reflect the quality of the characterization data on the NM and it is used for the similarity score and the overall quality score (not discussed in this Case).




**Constituents**: if the material is not pure, the other Constituents need to be defined. For this case, the concentration of TiO2 in the NM was 93 wt.% (from MSDS) and the remaining 7 wt.% were assumed to be Al2O3 and ZrO2, both with a concentration of 3.5 wt.%.

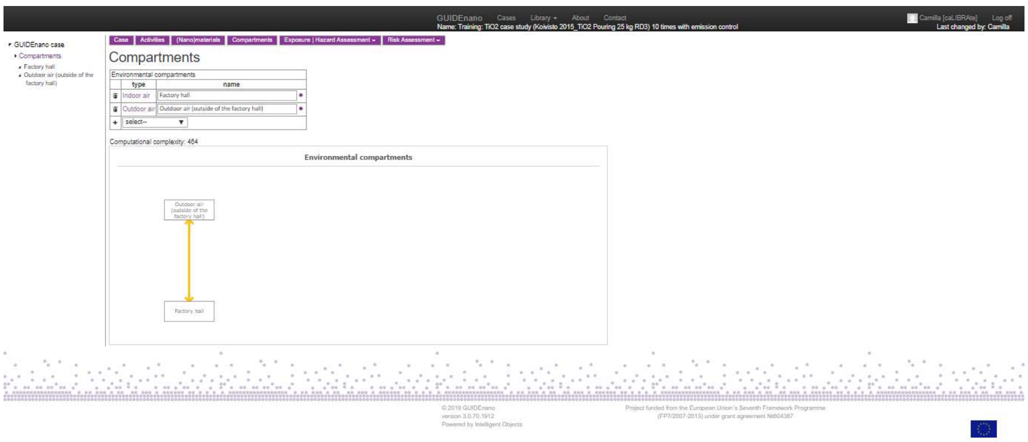



For each constituent defined, the user can provide further information such as chemical name, molecular formula, density and physical properties. To add/create a constituent the user has to select the kind of constituent (article, substance/mixture, nano-object, nanostructured aggregate or nanostructured agglomerate), and add constituent name, phase (ions, solid, liquid, gas), role (core, shell, coating, solid matrix, …), constituent concentration, unit, mass percent and hazard information. For each constituent, a tab appears with specific property groups to address. Which property groups are relevant depends on the category (material-class) used and its role. For a solid constituent, as a coating, the properties to fill will be: Identification, Physical properties of a chemical, Reactivity info, Classification & Labelling. These tabs request similar information as the one described before for the Physicochemical characteristic of the "entire" NM.

**Presence**: is automatically generated by the Tool once the user selects the relevant NM in the Compartments framework.

## Compartment framework

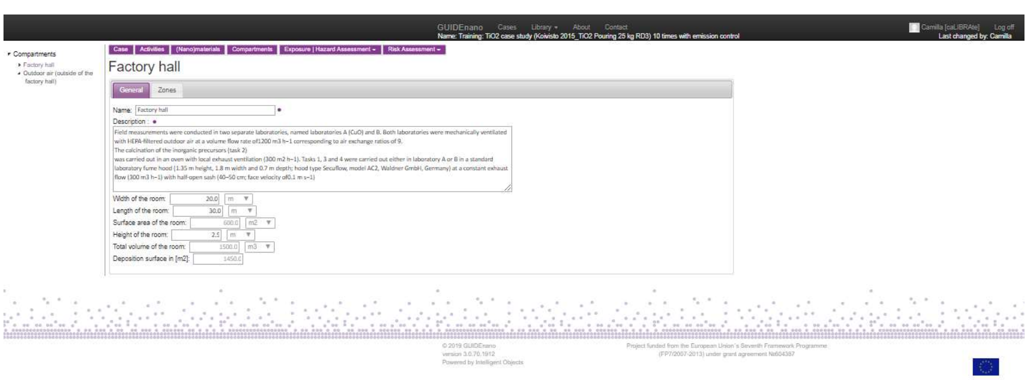
This framework is used to describe in which "system" or "environmental compartments" the released materials will first enter before getting in contact with the exposed species.



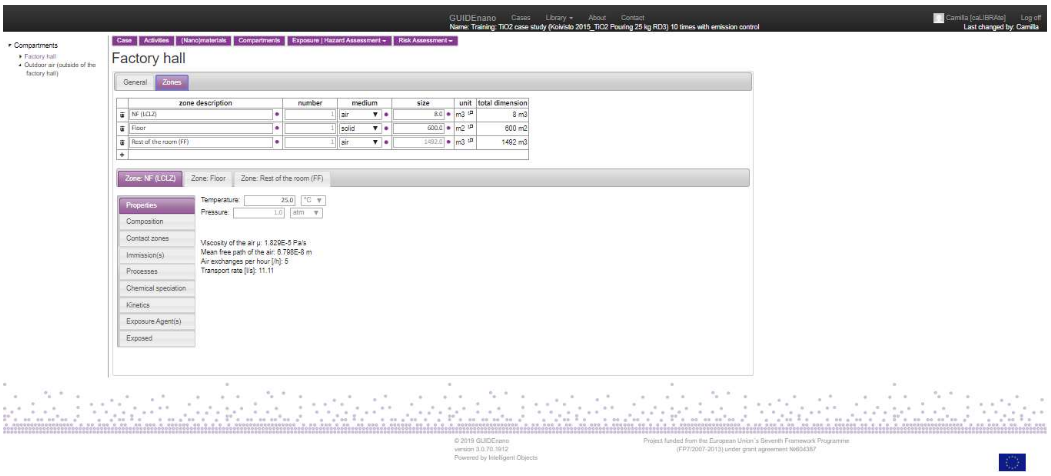

There are two groups of compartment type: the system compartment (which are manmade like as sewage system, waste water treatment plant, indoor air (room) and landfill site) and the environmental compartment (fresh water, estuarine, marine, fresh water sediment, salt water sediment, outdoor air and soil).

All compartments are organized in the same way, subdivided in General information and Zones.

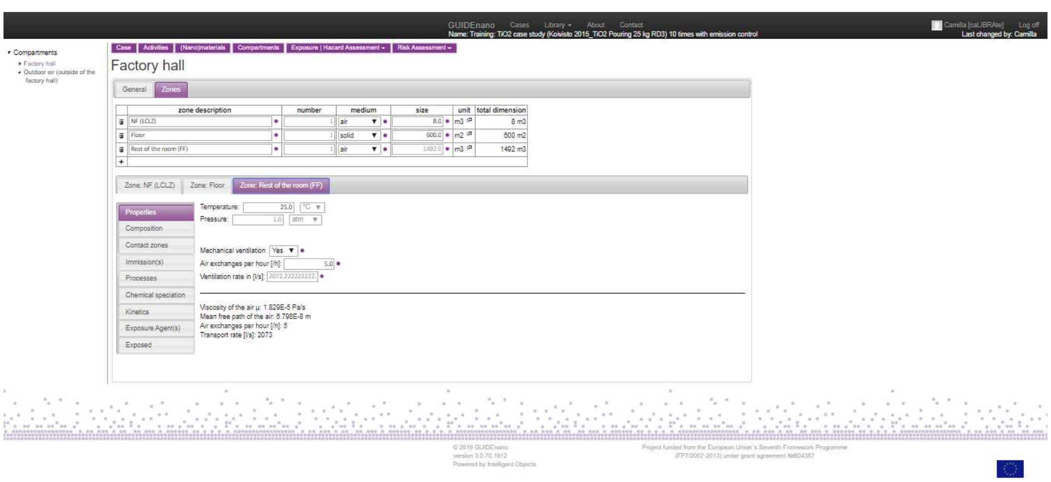
**General information**: for each compartment there are specific properties to fill. For example, in this case 2 compartments are defined, outdoor air and (Factory (indoor air)). For the compartment Factory Hall (indoor air), the user must enter a compartment name and a description and the room dimension (width, length, height of the room).



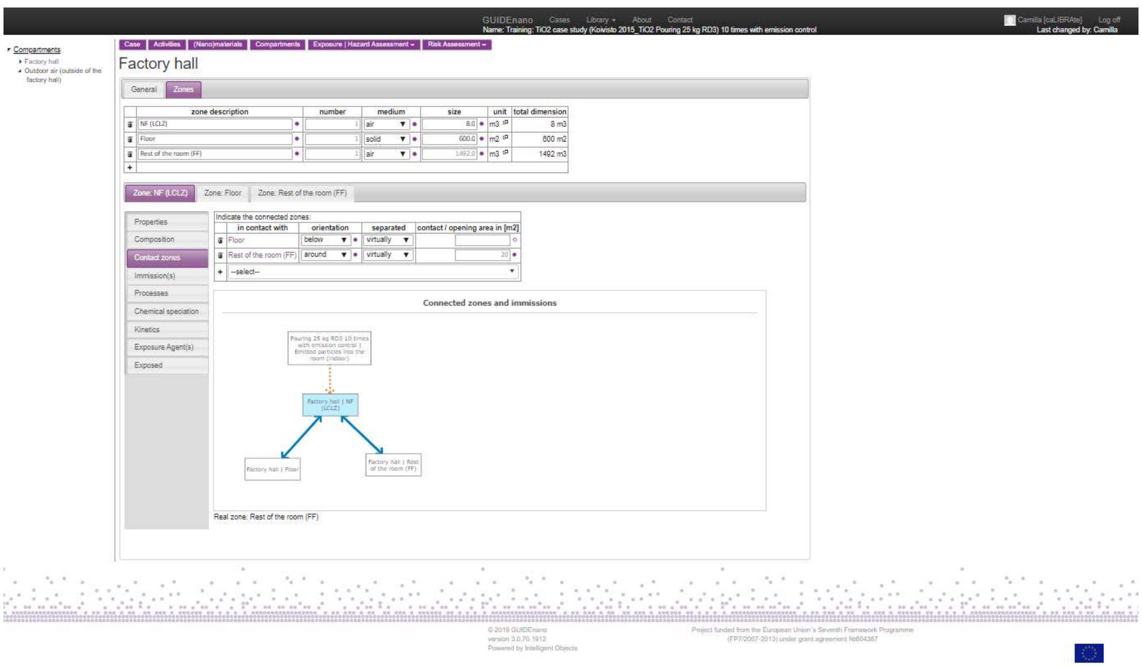
**Zones:** defines the different zones within the compartment. In this case, 2 compartments were defined, outdoor air and Factory (indoor air).



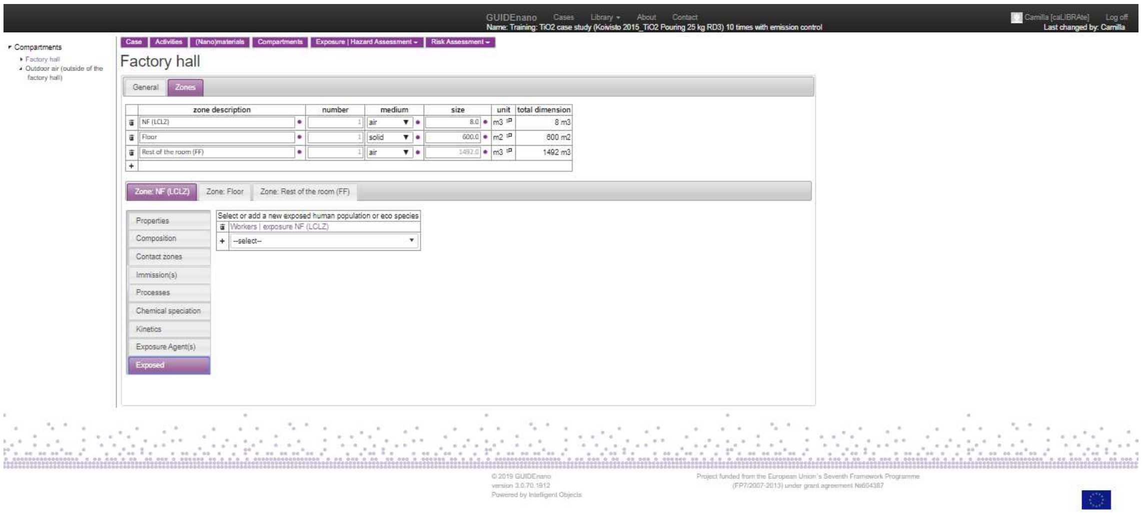

To define a zone, the user includes: zone description (NF, FF, floor, ...), number (number of identical zones within a compartment), medium (aquatic, solid, sediment, air), size and unit. The system compartment Factory Hall (indoor air) is divided in three different zones: 1) Zone description: NF (LCLZ), Number: 1, Medium: air, Size: 8 m3, 2) Zone description: Floor, Number: 1, Medium: solid, Size: 600 m2, 3) Zone description: FF (Rest of the room), Number: 1, Medium: air, Size: 1492 m3. For each zone added to the compartment, a separate tab is used to provide the zone-specific **Properties.** Depending on the selected medium, different properties become relevant, for an air medium (NF, FF) the temperature and the pressure are required. In addition, in the FF zone the air exchange per hour, which is 5 in the selected Case, is requested.



**Contact between zones:** the user can connect zones that are in contact, providing name of the zone “in contact with”, orientation (within, above, below, …), separation (virtually, physically) and contact/opening area between zones. Zones within the same compartment and between different compartments can be in contact. In the ES selected, the NF zone was in contact with “Floor, Orientation: below, Separated: virtually” and is in contact with “Rest of the Room (FF), Orientation: around, Separated: virtually”. The Floor zone is in contact with “NF (LCLZ), Orientation: above, Separated: virtually” and is in contact with “Rest of the Room (FF), Orientation: above, Separated: virtually”. The Rest of the Room (FF) zone is in contact with “NF (LCLZ), Orientation: within, Separated: virtually”, is in contact with “Floor, Orientation: below, Separated: virtually”.




**Exposed:** the user selects (or add) a new exposed human population (workers, consumers) or eco species that will be described in the Exposure framework. In the case of the ES considered, the workers are the exposed population.

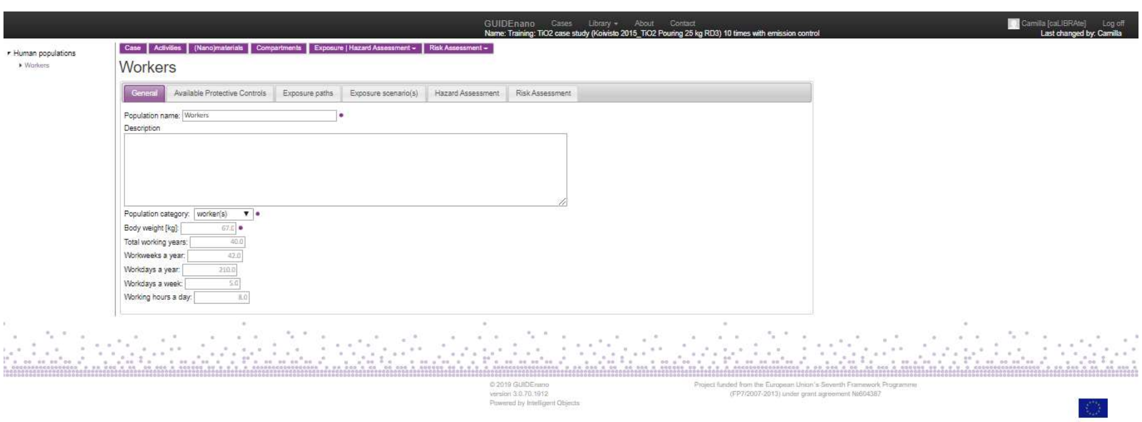



The remaining tabs (Composition, Immission(s), Processes, Chemical Speciation, Kinetics and Exposure Agent(s)) are automatically filled by the Tool according to the information previously used.

## Exposure framework and Hazard assessment framework

The exposure framework enables the user to define multiple exposure scenarios for both human populations and eco-populations throughout the entire product life cycle. The user can enter-in the exposed population selected in the "Exposed" tab in the Zone part or add an exposed population from this module.

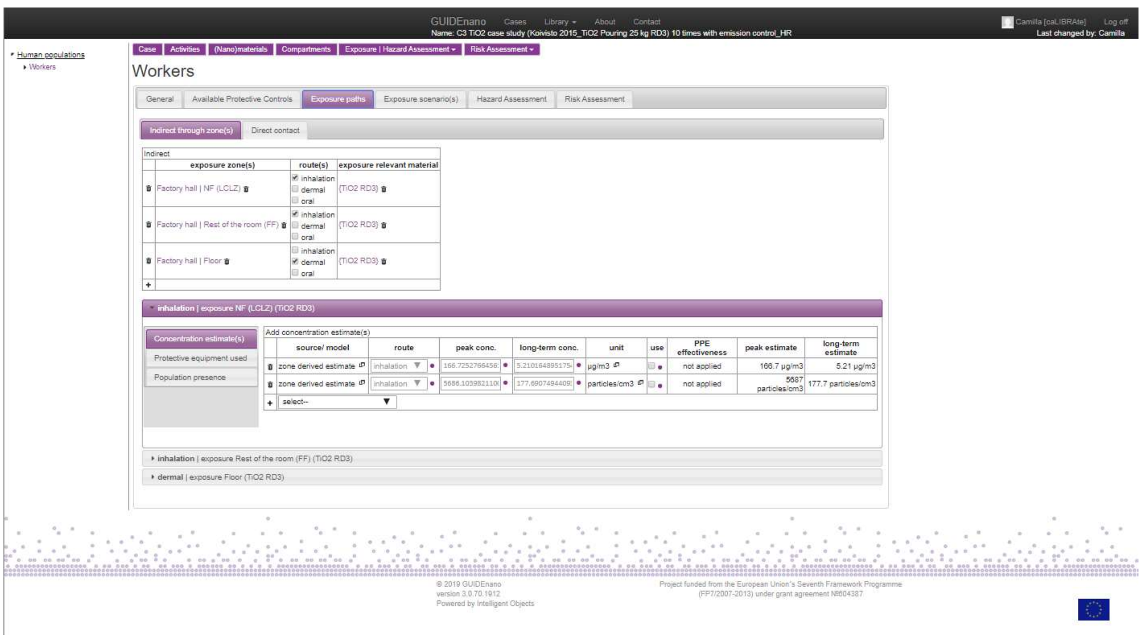

For human populations the user can fill in **General info**, such as the population name, description and category (workers, consumers, bystanders, etc.).




Moreover, body weight and information about working frequency can be provided, otherwise default values are used.

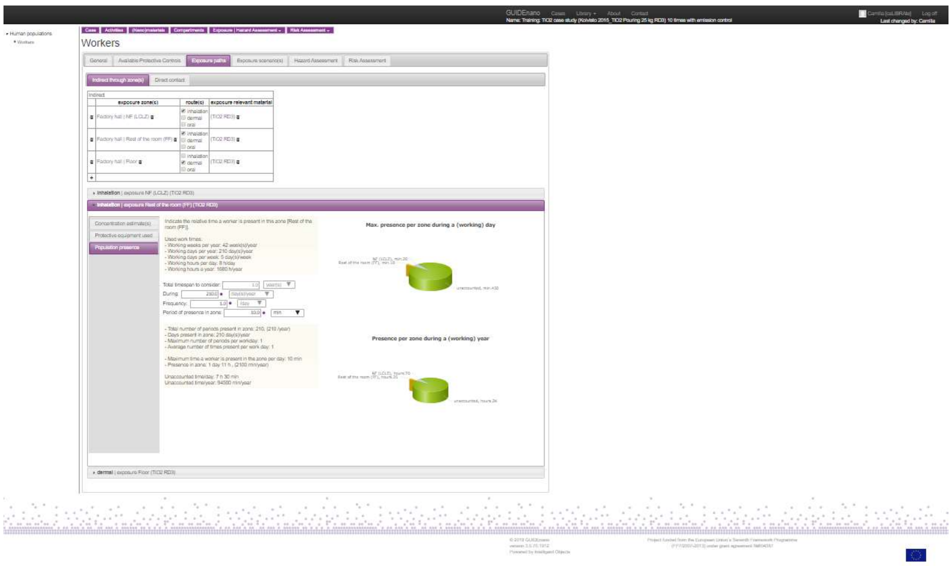
**Available Protective Controls:** In case of a worker population, the user can indicate which personnel protective equipment (PPE) is available at the work. If the PPEs is used the user need to enter this information in the following part (Protective Equipment tabs of the Indirect exposure (path)).

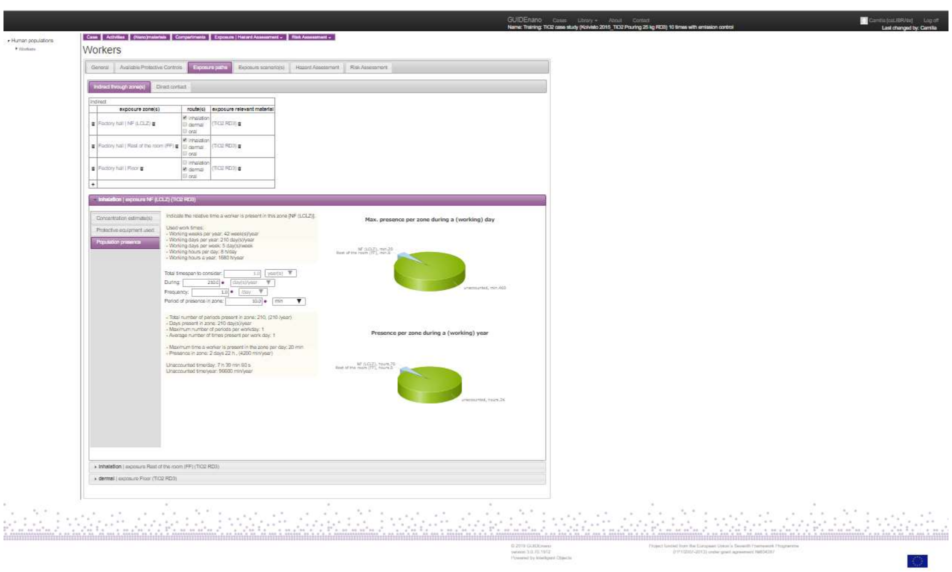
**Human exposure paths:** The tool supports both occupational and consumer exposure scenarios for three exposure routes: inhalation, dermal and oral. An exposure scenario is defined as a combination of one or more exposure paths related to the same exposure relevant (nano)material. Indirect exposure (path): When a population get in contact with the exposure relevant material due to its presence in the zone medium, the contact path is considered indirect, as in this case.




The user defines each indirect exposure paths selecting Exposure zone (Factory NF, Factory FF) and exposure Route (inhalation, dermal and oral), the tool indicates the corresponding Exposure relevant material. For each defined exposure path, the Concentration estimate(s) and the Protective Equipment can be defined. For the Concentration estimate(s) the user can select different methods and models to estimate the concentration of the exposure relevant material for a path. The user can also enter a user estimate or measured data. In the case of the ES selected, the worker exposure was indirect through the NF zone (by inhalation) and the exposure was derived from the Zone derived (fate model) estimate. By clicking on Use field, a thick appears and means that the value estimated will be used for the risk assessment. To pass to the following

Hazard assessment tab, the Population presence need to be filled for the exposure path(s) previously defined, depending on the presence of the worker in the zones. In this case, we assume that workers are present in NF and FF for 10 minutes each day, during 210 working days in 1 year. For this case we do not consider dermal exposure trough floor, as the workers are supposed to wear protective suits and shoes.

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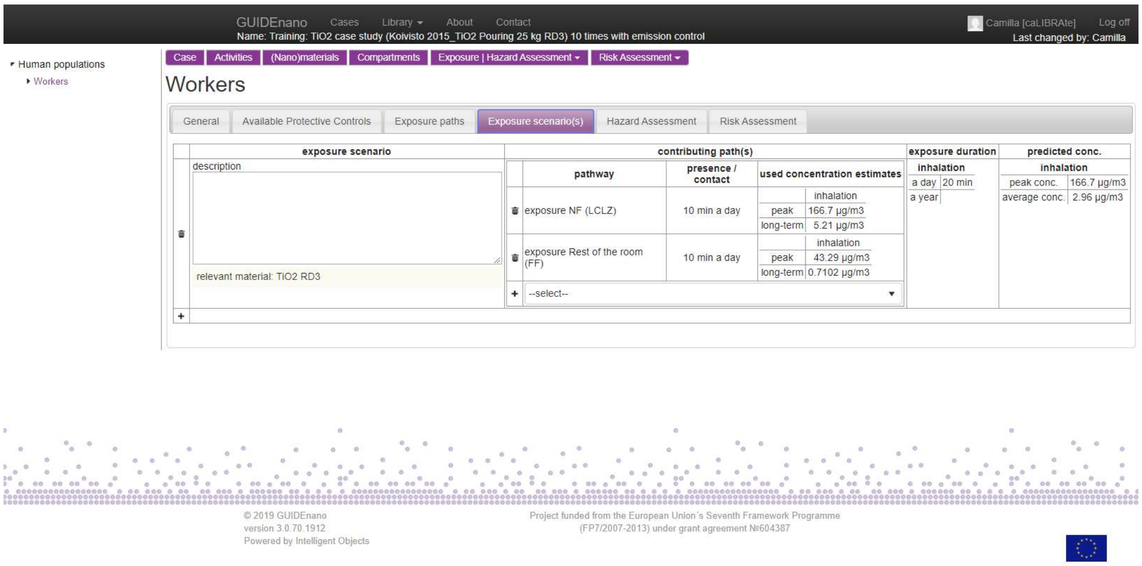
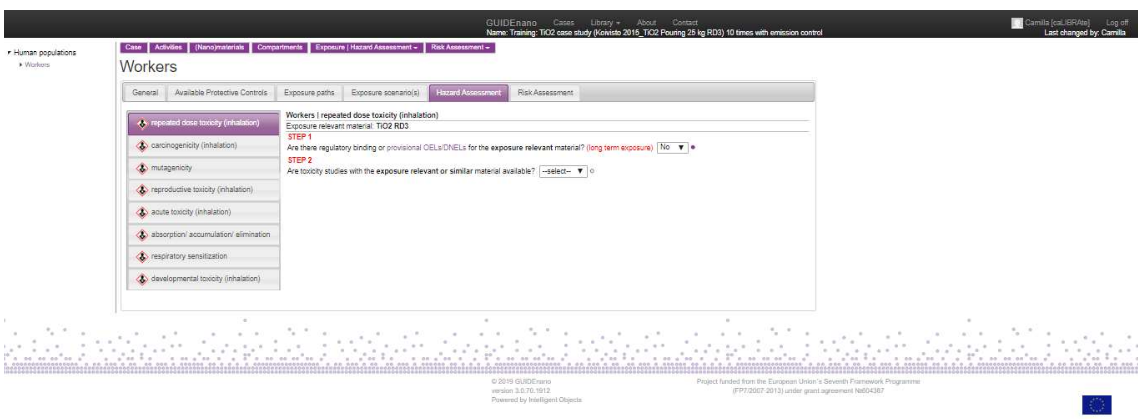
**Exposure scenario(s):** is generated by the user by clicking "+" and selecting the contributing path for the exposure. The Tool automatically report in the table the estimated concentration of the exposure relevant NM in the zones defined.




**Hazard assessment:** the following step to make the Hazard assessment is to have available a DNEL or OEL value for the relevant exposure NM and exposure path(s).




The Tool is asking the user if these values are available, in case they are not available the user can go through the similarity framework to estimate these values from a similar (nano)material. For this case, we have the OEL value available in the paper (Table 1) and user can select "yes" to the STEP 1 question. At this point, the user selects the Dose descriptors, the OEL in this case,

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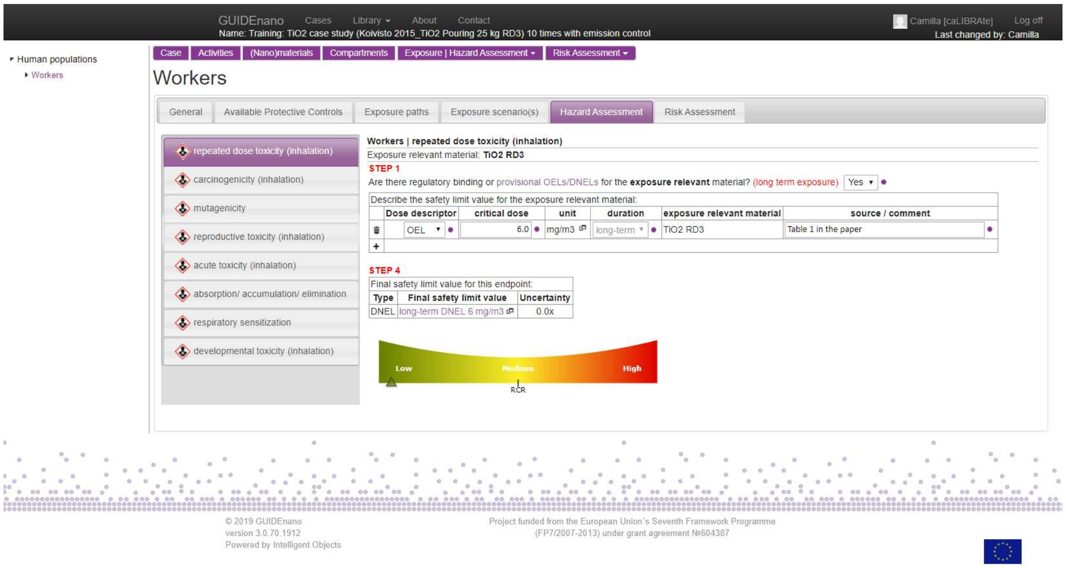
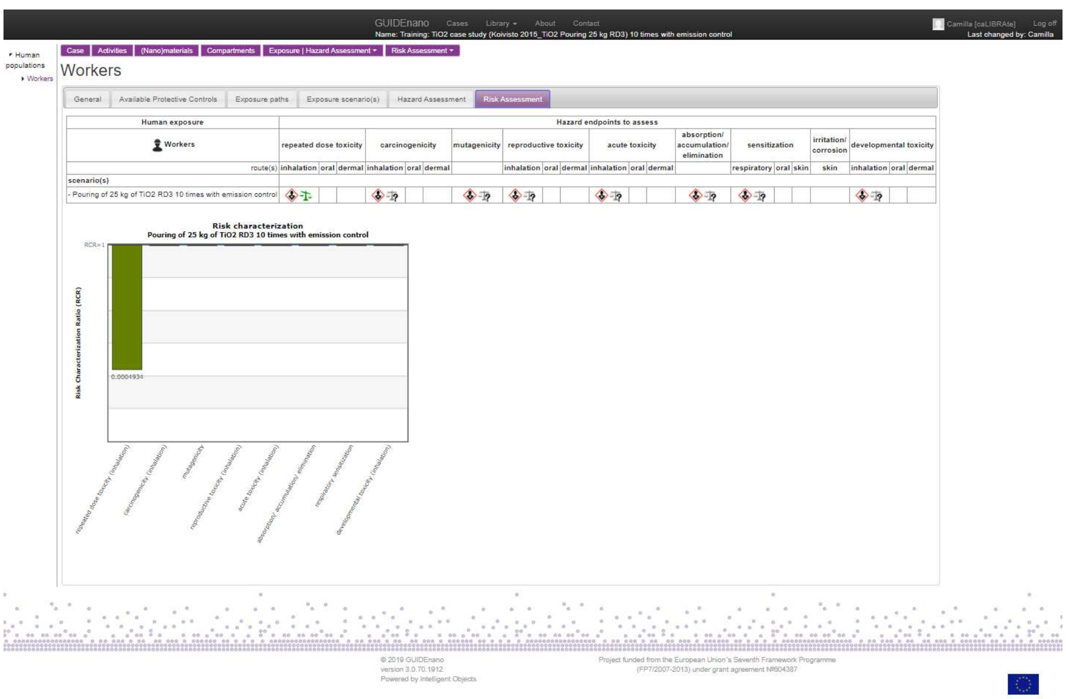
and the metrics to be used and fill-in the critical dose, that in this case is 6 mg/m3. Filling the critical dose entry, the user can obtain an indication of the Risk coefficient ratio (RCR).




**Risk assessment:** the Tool show an overview of the hazard endpoint considered with the corresponding RCR ratio reported also in a graph format.

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