

GUIDEnano

-

Example of Use in “Pouring small bags of TiO₂ powder” case study

Authors and reviewers <i>[Add lines if needed]</i>			
Full Name	Beneficiary	E-mail	Role
Camilla Delpivo	LEITAT	cdelpivo@leitat.org	Lead Author
			Contributor
			Contributor
			Contributor
Socorro Vazquez-Campos	LEITAT	svazquez@leitat.org	Reviewer
			Reviewer
			Reviewer

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1.0			First draft
			First revision
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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 TiO₂ 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)]

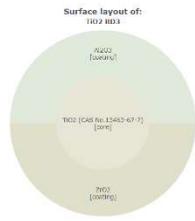
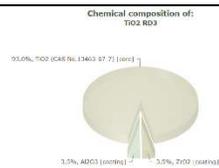
Most of the input parameters needed to model this Case study, including the work environment, the process information and the NM characteristics, are provided from the literature paper. The table below report the input parameters required by GUIDEnano, indicating which data entry are recommended (R) 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



32	Average formula mass in [g/mol]:	79.8658	Automatically calculated.
33	Density:	4.0 g/cm ³	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:	Al ₂ O ₃	R
38	Molecular formula:	Al ₂ O ₃	M
39	Average 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:	ZrO ₂	R
44	Molecular formula:	ZrO ₂	M
45	Average 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 TiO ₂ nanomaterial poured during the activity, Material: TiO ₂ 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. 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. 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. In contact with: Floor , Orientation: below, Separated: virtually. 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



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” (TiO₂ 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 Coefficient 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.



I. Annex I

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

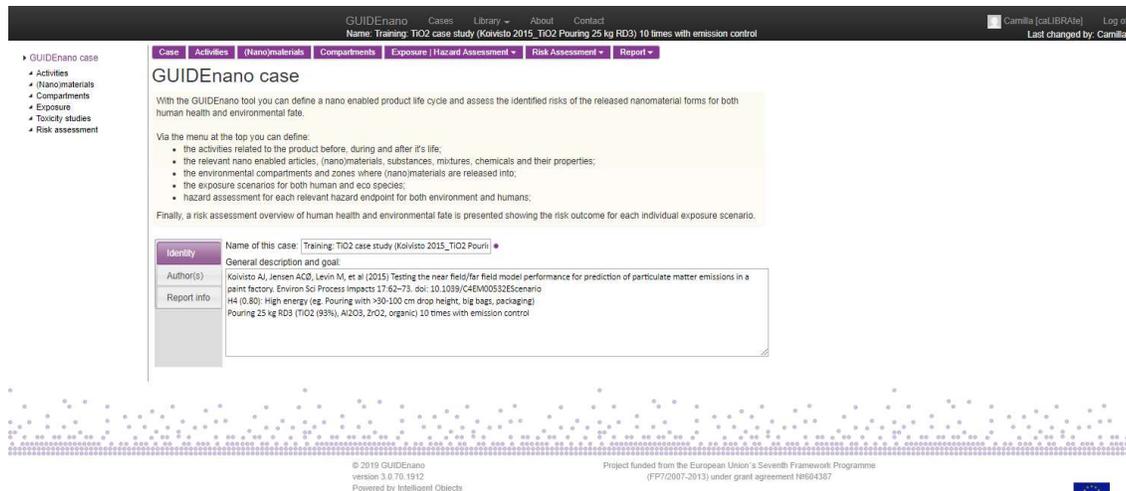
GUIDEnano Case from the literature paper published on Environ. Sci. Process. Impacts 17:62–73. doi: 10.1039/C4EM00532E Scenario “Testing the near field/far field model performance for prediction of particulate matter emissions in a paint factory”, Koivisto AJ, Jensen ACØ, Levin M, et al (2015).

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.



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/C4EM00532ESscenario”, 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.



The screenshot shows the GUIDEnano web application interface. At the top, there is a navigation bar with the following items: GUIDEnano, Cases, Library, About, Contact, Camilla (caLIBRAte), and Log off. Below the navigation bar, there is a breadcrumb trail: Case > Activities > (Nano)materials > Compartments > Exposure > Hazard Assessment > Risk Assessment > Report. The main content area is titled "GUIDEnano case" and contains the following text:

With the GUIDEnano tool you can define a nano enabled product life cycle and assess the identified risks of the released nanomaterial forms for both human health and environmental fate.

Via the menu at the top you can define:

- the activities related to the product before, during and after it's life;
- the relevant nano enabled articles, (nano)materials, substances, mixtures, chemicals and their properties;
- the environmental compartments and zones where (nano)materials are released into;
- the exposure scenarios for both human and eco species;
- hazard assessment for each relevant hazard endpoint for both environment and humans;

Finally, a risk assessment overview of human health and environmental fate is presented showing the risk outcome for each individual exposure scenario.

The interface also shows a form with the following fields:

- Identity:** Name of this case: Training: TiO2 case study (Koivisto 2015_TiO2 Pouring)
- 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/C4EM00532ESscenario
- Author(s):** Hi (I, B): High energy (eg. Pouring with 300-100 cm drop height, big bags, packaging)
- Report info:** Pouring 25 kg RD3 (TiO2 (93%), Al2O3, ZnO, organic) 10 times with emission control

At the bottom of the page, there is a footer with the following information:

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Project funded from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement 14964307



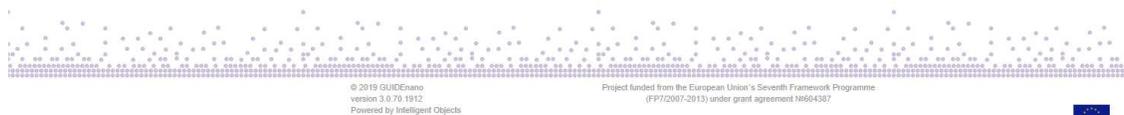
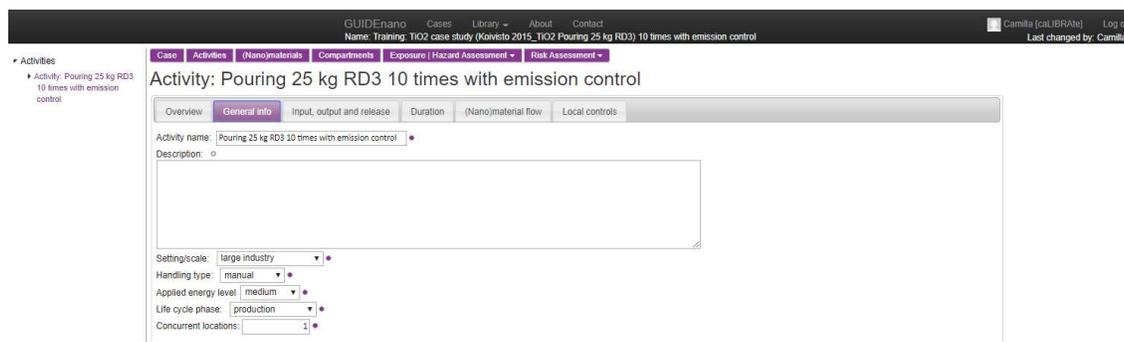

Activities

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.



GUIDEnano Cases Library About Contact
Name: C3 TiO2 case study (Kovisto 2015_TiO2 Pouring 25 kg RD3) 10 times with emission control_HR
Camilla [caLIBRAte] Log off
Last changed by: Camilla

Case Activities (Nano)materials Compartments Exposure Hazard Assessment Risk Assessment

Activities
Activity: Pouring 25 kg RD3 10 times with emission control

Activity: Pouring 25 kg RD3 10 times with emission control

Overview General info **Input, output and release** Duration (Nano)material flow Local controls

Activity input

input description	material	relative to	relative amount	total amount	unit	ref.	rate
TiO2 nanomaterials that are poured during the acti...	TiO2 RD3			250.0	kg		25 kg/min

Activity output(s)

output description	material	relative to	relative amount	total amount	unit	ref.	rate
TiO2 contained in the formulated paint	TiO2 RD3	input TiO2 nanomaterials that are poured during the activity	100 %	249.998675	kg		

Activity release(s)

release description	released material	relative to	relative release	RMM's	total release	unit	ref.	rate/location
Emitted particles into the room (indoor)	TiO2 RD3	input TiO2 nanomaterials that are poured during the activity	0.00053 % /cycle	90.0%	0.0001323	kg		13.25 mg/min

Overall mass balance [output(s) + release(s)] / input: 1
The total [output + release] of nano-constituent [TiO2 RD3] is less than its [input] 0.000477 % unaccounted mass!

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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),

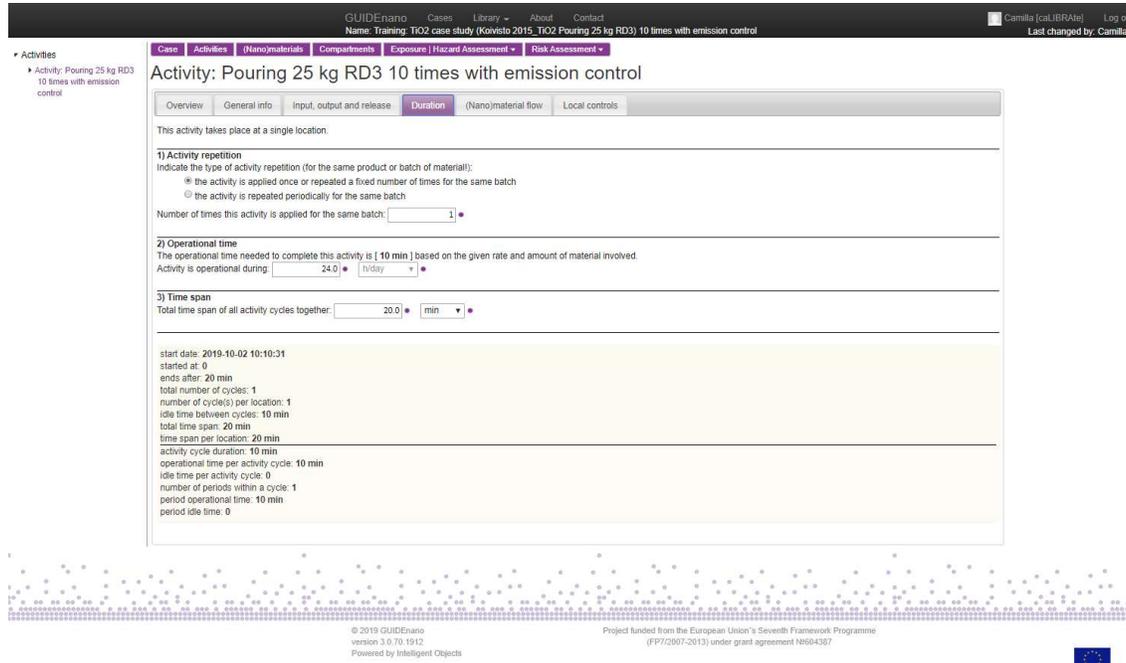


relative amount (it is the amount of released material relative to the input material), risk mitigation measures (RMM's), total release, unit, reference, rate/location, describing the release rate per location. Internal mass flow: the connectors are also used to define the internal and the external mass 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 TiO₂ nanomaterial (TiO₂ RD3) poured during the activity, the total amount is 250 kg with a (pouring) rate of 25 kg/min. The Activity output is the TiO₂ (TiO₂ 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 TiO₂ 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).



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!).



Activity: Pouring 25 kg RD3 10 times with emission control

1) Activity repetition
Indicate the type of activity repetition (for the same product or batch of material!):
 the activity is applied once or repeated a fixed number of times for the same batch
 the activity is repeated periodically for the same batch
 Number of times this activity is applied for the same batch:

2) Operational time
The operational time needed to complete this activity is based on the given rate and amount of material involved.
 Activity is operational during: h/day

3) Time span
Total time span of all activity cycles together: min

start date:	2019-10-02 10:10:31
started at:	0
ends after:	20 min
total number of cycles:	1
number of cycle(s) per location:	1
idle time between cycles:	10 min
total time span:	20 min
time span per location:	20 min
activity cycle duration:	10 min
operational time per activity cycle:	10 min
idle time per activity cycle:	0
number of periods within a cycle:	1
period operational time:	10 min
period idle time:	0

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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.

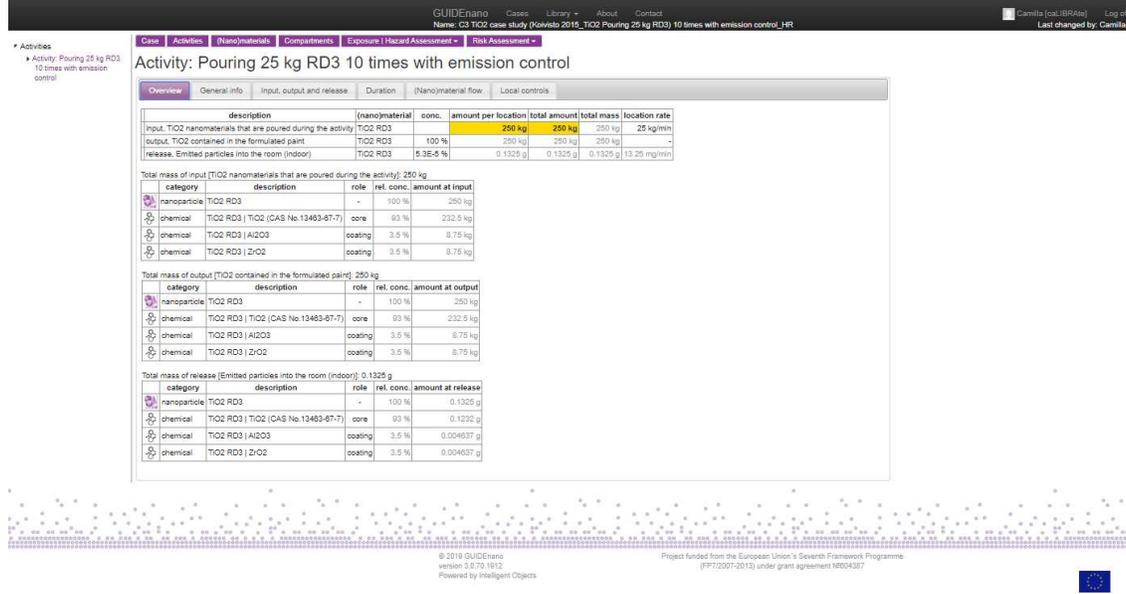


The screenshot shows the 'Local controls' tab in the GUIDEnano software. The activity is 'Pouring 25 kg RD3 10 times with emission control'. A table lists the local controls:

mitigation of release	redirected towards	efficacy value	already accounted	active
Fume hood (standard, exhaust flow 704.7 m3/h) release Emitted particles into the room (indoor)	an output	0.9	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Below the table is a 'Local control wizard' button.

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



The screenshot shows the '(Nano)material flow' tab in the GUIDEnano software. It displays a summary table and detailed breakdowns of input, output, and release.

description	(nano)material	conc.	amount per location	total amount	total mass	location rate
input, TiO2 nanomaterials that are poured during the activity	TiO2 RD3	-	250 kg	250 kg	250 kg	25 kg/min
output, TiO2 contained in the formulated paint	TiO2 RD3	100 %	250 kg	250 kg	250 kg	-
release, Emitted particles into the room (indoor)	TiO2 RD3	5.3E-4 %	0.1325 g	0.1325 g	0.1325 g	13.25 mg/min

Total mass of input (TiO2 nanomaterials that are poured during the activity): 250 kg

category	description	role	rel. conc.	amount at input
nanoparticle	TiO2 RD3	-	100 %	250 kg
chemical	TiO2 RD3 TiO2 (CAS No. 13493-67-7)	core	93 %	232.5 kg
chemical	TiO2 RD3 Al2O3	coating	3.5 %	8.75 kg
chemical	TiO2 RD3 ZrO2	coating	3.5 %	8.75 kg

Total mass of output (TiO2 contained in the formulated paint): 250 kg

category	description	role	rel. conc.	amount at output
nanoparticle	TiO2 RD3	-	100 %	250 kg
chemical	TiO2 RD3 TiO2 (CAS No. 13493-67-7)	core	93 %	232.5 kg
chemical	TiO2 RD3 Al2O3	coating	3.5 %	8.75 kg
chemical	TiO2 RD3 ZrO2	coating	3.5 %	8.75 kg

Total mass of release (Emitted particles into the room (indoor)): 0.1325 g

category	description	role	rel. conc.	amount at release
nanoparticle	TiO2 RD3	-	100 %	0.1325 g
chemical	TiO2 RD3 TiO2 (CAS No. 13493-67-7)	core	93 %	0.1232 g
chemical	TiO2 RD3 Al2O3	coating	3.5 %	0.004637 g
chemical	TiO2 RD3 ZrO2	coating	3.5 %	0.004637 g



GUIDEnano Case Library About Contact
Name: Training: TiO2 case study (Kowello 2015_TiO2 Pouring 25 kg RD3) 10 times with emission control

Home (caLIBRAte) Log off
Last changed by: Camilla

Case: Activities (Nano)materials Compartments Exposure Hazard Assessment Risk Assessment

Activity: Pouring 25 kg RD3 10 times with emission control

Overview General info Input, output and release Duration (Nano)material flow Local controls

input from preceding activity transport time unit
TiO2 nanomaterials that are poured during the activity connect ID

output(s) to succeeding activity transport time unit
TiO2 contained in the formulated paint connect ID

release(s) into compartment | zone or directly in contact with
release | Emitted particles into the room (indoor) Factory hall | NF (LCLZ)

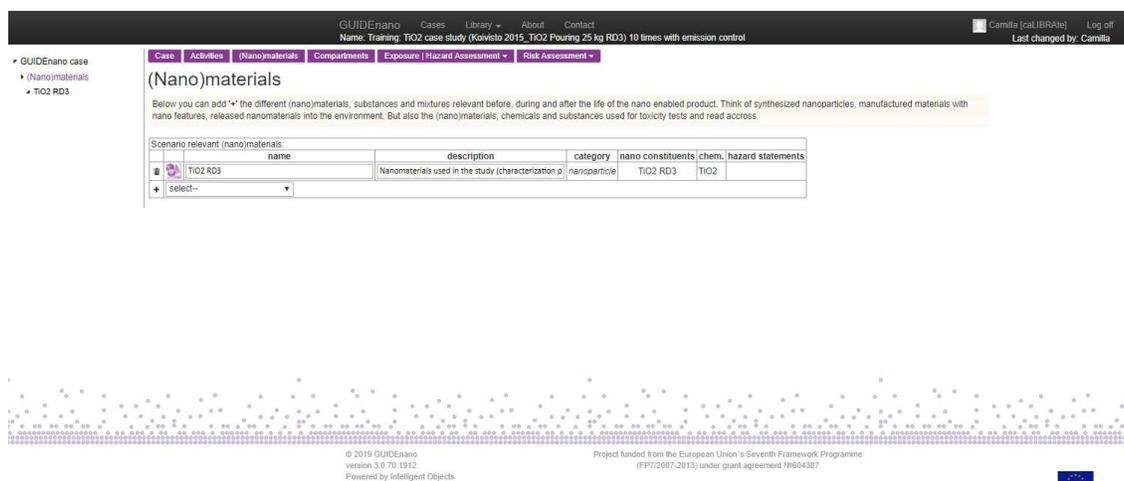
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version 3.0.79: 8942
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Project funded from the European Union's Seventh Framework Programme
(FP7/2007-2013) under grant agreement N6646307



(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.



The screenshot shows the GUIDEnano web application interface. At the top, there is a navigation bar with 'GUIDEnano' and links for 'Cases', 'Library', 'About', and 'Contact'. Below this, the current case is identified as 'Name: Training: TiO2 case study (Kovisto 2015, TiO2 Pouring 25 kg RD3) 10 times with emission control'. The user is logged in as 'Camilla (caLIBRAte)' and the last change was made by 'Camilla'. The main navigation tabs include 'Case', 'Activities', '(Nano)materials', 'Compartments', 'Exposure', 'Hazard Assessment', and 'Risk Assessment'. The '(Nano)materials' tab is active, showing a table for 'Scenario relevant (nano)materials'.

name	description	category	nano constituents	chem.	hazard statements
TiO2 RD3	Nanomaterials used in the study (characterization p	nanoparticle	TiO2 RD3	TiO2	

Below the table, there is a 'select--' dropdown menu. At the bottom of the page, there is a decorative pattern of dots and a footer containing copyright information: '© 2019 GUIDEnano version 3.0.70.1912 Powered by Intelligent Objects' and 'Project funded from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement N6604357'. The European Union flag is also present in the footer.

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.



GUIDEnano Case Library About Contact
Name: Training: TiO2 case study (Kovisto 2015, TiO2 Pouring 25 kg RD3) 10 times with emission control

Camilla (caLIBRAte) Log off
Last changed by: Camilla

Case Activities (Nanomaterials) Compartments Exposure Hazard Assessment Risk Assessment

(Nanomaterials) → TiO2 RD3

TiO2 RD3

Physico-chemical characteristics Constituents(3) Presence(3)

Nanomaterial category: nanoparticle

Identification

Shape and size Morphology / shape: spherical

Physical properties Mean size

Surface properties Mean nanoscaled particle diameter (D1 - D2 - D3) in nm: 0

Function(s) Aspect ratio: 1.0

Mass conversion Size method/distribution

Chemical info Size distribution data available? Yes

Reactivity info Method used: Other Size type: primary size

Classification & Labelling

Toxicity studies

Quality: (88.0%)

Size distribution

Metric: (Mass based) Distribution: (Normal) Mean size in nm: 220 Standard deviation: 22.0

Primary size distribution diameter	%	g/gram	#bin	#g_bin	g_bin#	m2/g	mass%	number%
0 - 1nm	0.0	0	0	0	0	1.04E-21	1890	0%
1 - 10nm	0.0	0	0	0	0	0.8E0017	1.04E-19	188.9
10 - 30nm	0.0	0	0	0	0	3.4E0016	2.93E-17	62.24
30 - 100nm	0.0	0	0	0	0	3.8E0014	1.07E-15	18.73
100 - 300nm	100.0	1	3	4	3	2.93E-14	6.224	100%
300 - 500nm	0.0	0	0	0	0	8.3E0012	1.56E-13	3.841
500 - 1000nm	0.0	0	0	0	0	8.8E0011	1.17E-12	1.817
1000 - 3000nm	0.0	0	0	0	0	3.4E0010	2.93E-11	0.8324
3000 - 10000nm	0.0	0	0	0	0	3.8E0009	1.56E-10	0.3541
10000 - 100000nm	0.0	0	0	0	0	8.8E0008	1.17E-09	0.1817
100000nm+	0.0	0	0	0	0	928.0	0.001078	0.001871

Particle density: 4 g/cm³
 Particles per gram: 3.4E+13 particles/g [TiO2 RD3]
 Average mass per particle: 2.93E-14 g/particle [TiO2 RD3]
 Surface area per gram: 6.224 m²/g [TiO2 RD3]
 Average volume based size: 342 nm
 Percentage of particles in nanoscale: 0 %

Size distribution graph showing mass based (blue) and number based (yellow) distributions. The x-axis is size bins (0-1nm to 100000nm+) and the y-axis is % (0-100%).

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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.

GUIDEnano Case Library About Contact
Name: Training: TiO2 case study (Kovisto 2015, TiO2 Pouring 25 kg RD3) 10 times with emission control

Camilla (caLIBRAte) Log off
Last changed by: Camilla

Case Activities (Nanomaterials) Compartments Exposure Hazard Assessment Risk Assessment

(Nanomaterials) → TiO2 RD3

TiO2 RD3

Physico-chemical characteristics Constituents(3) Presence(3)

Nanomaterial category: nanoparticle

Identification Physical state of this material: solid

Shape and size Indicate the size category(s) this solid material may present itself:

Physical properties solid object (> 10 nm) broken solid (3 - 10 nm) granular solid (0.1 - 3 mm) granular powder (10 - 100 µm) asperine powder (1 - 10 µm) ultrafine powder (100 nm - 1 µm) nanoscaled particles (1 nm - 100 nm)

Surface properties Rigidity: 0.01

Function(s) Dustiness (mg/kg): 0.3

Mass conversion Melting point in °C: 0

Chemical info Boiling point in °C: 0

Reactivity info

Classification & Labelling

Toxicity studies

Quality: (88.0%)

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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.

The screenshot shows the 'Surface properties' section of the caLIBRAte software. The 'Layout and charge' table is as follows:

chemical compound	role	contact order	surface charge	Zeta potential	medium	solubility	hydrophobicity/hydrophilicity
TiO2 (CAS No. 13463-67-7)	core	1				insoluble	
A203	coating	2	Positive	> +25 mV	pH	insoluble	hydrophobic
ZnO2	coating	2	Positive	> +25 mV	pH	insoluble	hydrophobic

The 'Surface layout' pie chart shows the relative proportions of the constituents: TiO2 (CAS No. 13463-67-7) at 71%, ZnO2 (100%) at 29%, and A203 (100%) at 0%.

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

The screenshot shows the 'Functions' section of the caLIBRAte software. The 'Indicate the function(s)' list includes:

- binder
- pigment
- UV filter
- antimicrobial agent
- conductor
- preservative
- catalyst
- photocatalyst
- wetting agent
- self-cleaning agent
- thickening agent
- anticaking agent
- reinforcing filler
- other

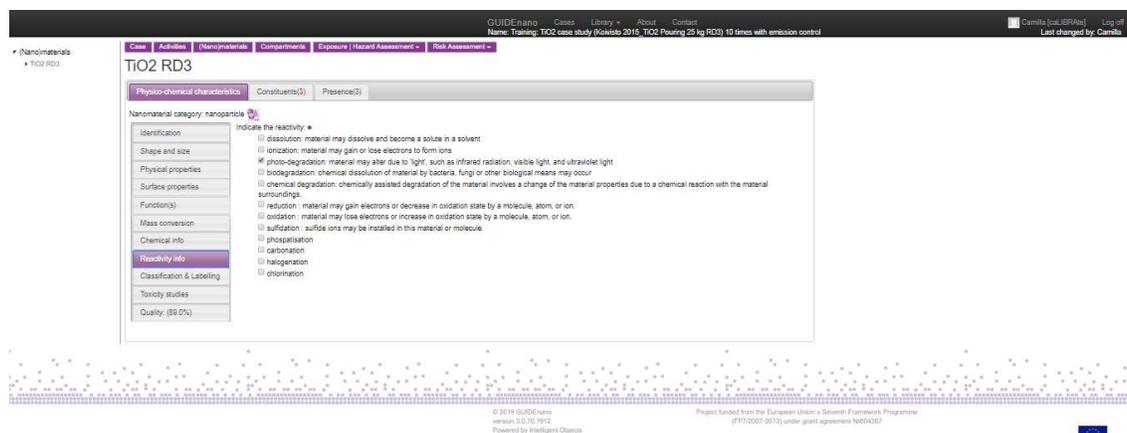


Mass conversion: The user can select different mass conversion metrics (mole, particle number, volume, surface area, ...).

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



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



GUIDEnano Cases Library About Contact
Name: Training: TiO2 case study (Kicikids 2015- TiO2 Posing 25 kg RD3) 10 times with emission control
Camilla [out, ERF/Ita] Log off
Last changed by: Camilla

(Nano)materials
TiO2 RD3

Case Activities (Nano)materials Compartments Exposure Hazard Assessment Risk Assessment

Physico-chemical characteristics Constituents(3) Presence(3)

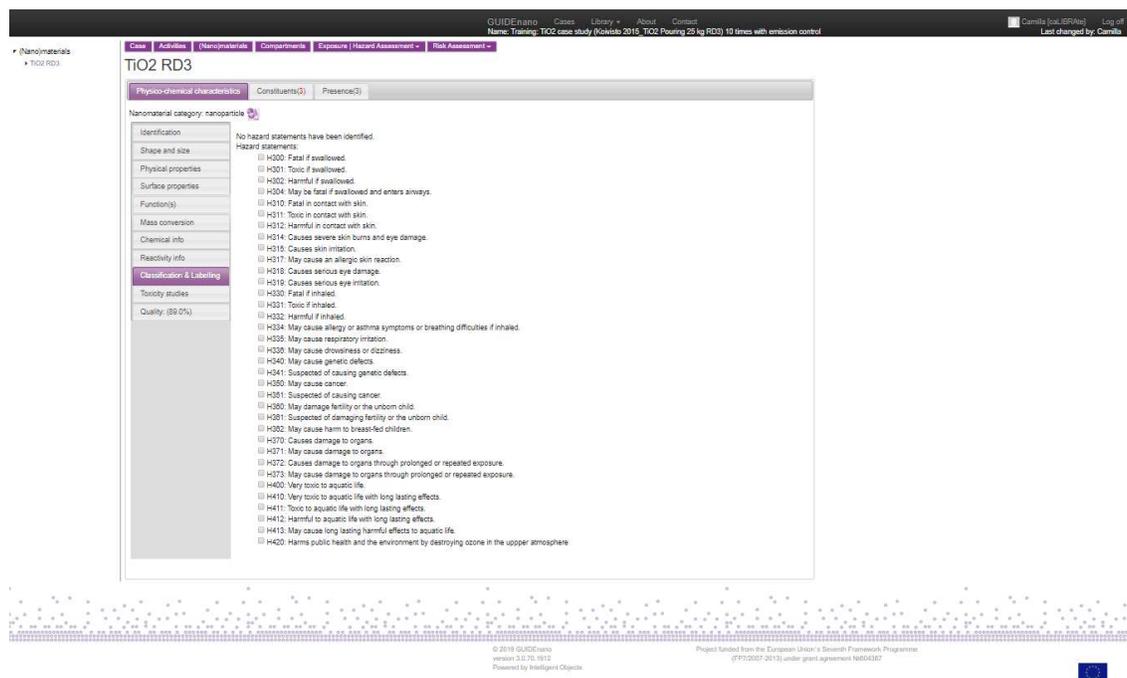
Nanomaterial category: nanoparticle

Indicate the reactivity

- dissolution: material may dissolve and become a solute in a solvent
- ionization: material may gain or lose electrons to form ions
- photo-degradation: material may alter due to 'light', such as infrared radiation, visible light, and ultraviolet light
- biological degradation: chemical dissolution of material by bacteria, fungi or other biological means may occur
- chemical degradation: chemically assisted degradation of the material involves a change of the material properties due to a chemical reaction with the material surroundings
- reduction: material may gain electrons or decrease in oxidation state by a molecule, atom, or ion
- oxidation: material may lose electrons or increase in oxidation state by a molecule, atom, or ion
- sulfidation: sulfide ions may be installed in this material or molecule
- phosphatization
- cationation
- halogenation
- chlorination

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



GUIDEnano Cases Library About Contact
Name: Training: TiO2 case study (Kicikids 2015- TiO2 Posing 25 kg RD3) 10 times with emission control
Camilla [out, ERF/Ita] Log off
Last changed by: Camilla

(Nano)materials
TiO2 RD3

Case Activities (Nano)materials Compartments Exposure Hazard Assessment Risk Assessment

Physico-chemical characteristics Constituents(3) Presence(3)

Nanomaterial category: nanoparticle

No hazard statements have been identified.

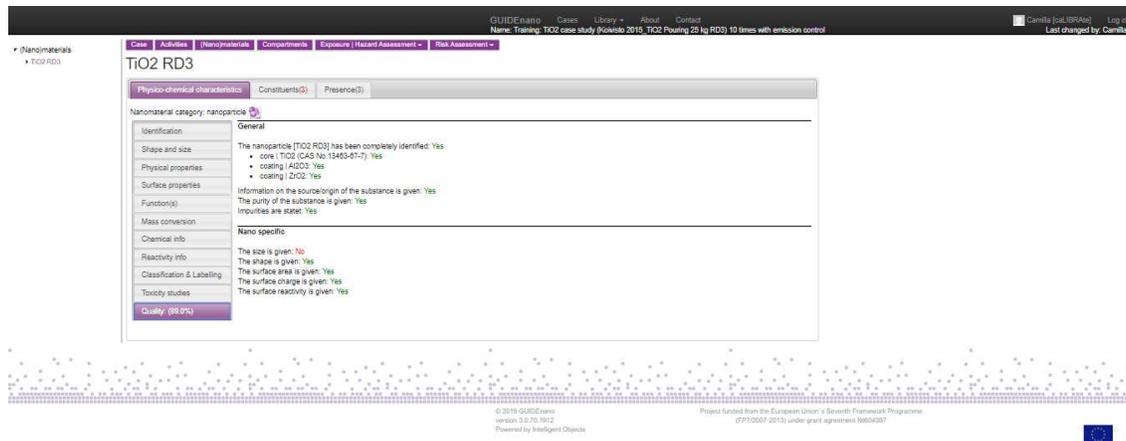
Hazard statements:

- H300: Fatal if swallowed
- H301: Toxic if swallowed
- H302: Harmful if swallowed
- H304: May be fatal if swallowed and enters airways
- H310: Fatal in contact with skin
- H311: Toxic in contact with skin
- H312: Harmful in contact with skin
- H314: Causes severe skin burns and eye damage
- H315: Causes skin irritation
- H317: May cause an allergic skin reaction
- H318: Causes serious eye damage
- H319: Causes serious eye irritation
- H330: Fatal if inhaled
- H331: Toxic if inhaled
- H332: Harmful if inhaled
- H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled
- H335: May cause respiratory irritation
- H336: May cause drowsiness or dizziness
- H340: May cause genetic defects
- H341: Suspected of causing genetic defects
- H350: May cause cancer
- H351: Suspected of causing cancer
- H360D: May damage fertility or the unborn child
- H361: Suspected of damaging fertility or the unborn child
- H362: May cause harm to breast-fed children
- H370: Causes damage to organs
- H371: May cause damage to organs
- H372: Causes damage to organs through prolonged or repeated exposure
- H373: May cause damage to organs through prolonged or repeated exposure
- H400: Very toxic to aquatic life
- H410: Very toxic to aquatic life with long lasting effects
- H411: Toxic to aquatic life with long lasting effects
- H412: Harmful to aquatic life with long lasting effects
- H413: May cause long lasting harmful effects to aquatic life
- H420: Harms public health and the environment by destroying ozone in the upper atmosphere

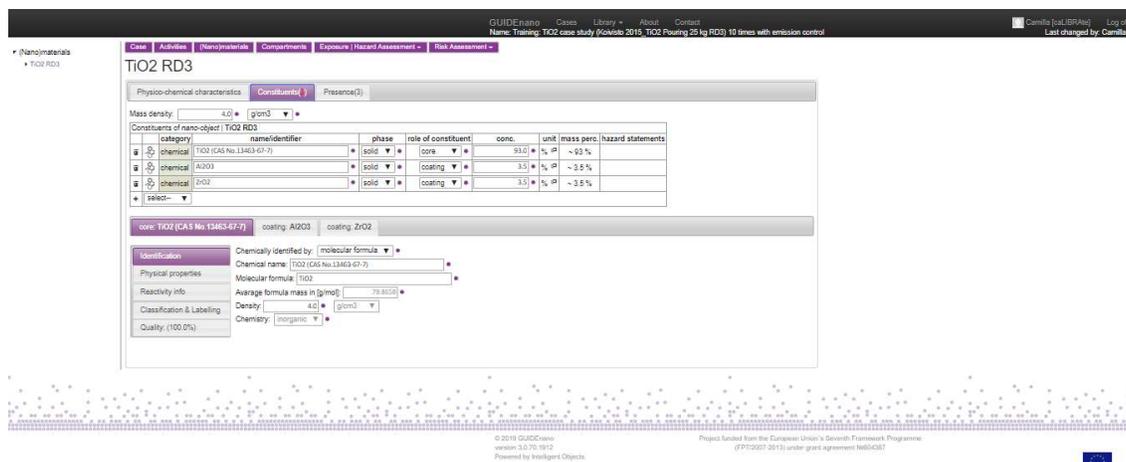
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Quality: for the Hazard assessment, if toxicity data on relevant NM and endpoint (such as DNEL or OEL for inhalation exposure) are not available, the user can add Toxicity study related to the relevant NM or related to a similar NM. The Quality score 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.



The screenshot displays the GUIDEnano web application interface. At the top, there is a navigation bar with links for 'GUIDEnano', 'Cases', 'Library', 'About', and 'Contact'. A user profile 'Camilla [caLIBRAte]' is logged in, with the last change by 'Camilla'. The main navigation menu includes 'Case', 'Activities', 'Nanomaterials', 'Compartments', 'Exposure | Hazard Assessment', and 'Risk Assessment'. The current view is for a 'Case' titled 'TiO2 RD3'. The interface shows a sidebar with '(Nanomaterials)' and 'TiO2 RD3'. The main content area has tabs for 'Physico-chemical characteristics', 'Constituents(3)', and 'Presence(3)'. The 'Presence(3)' tab is active, showing a table with the following data:

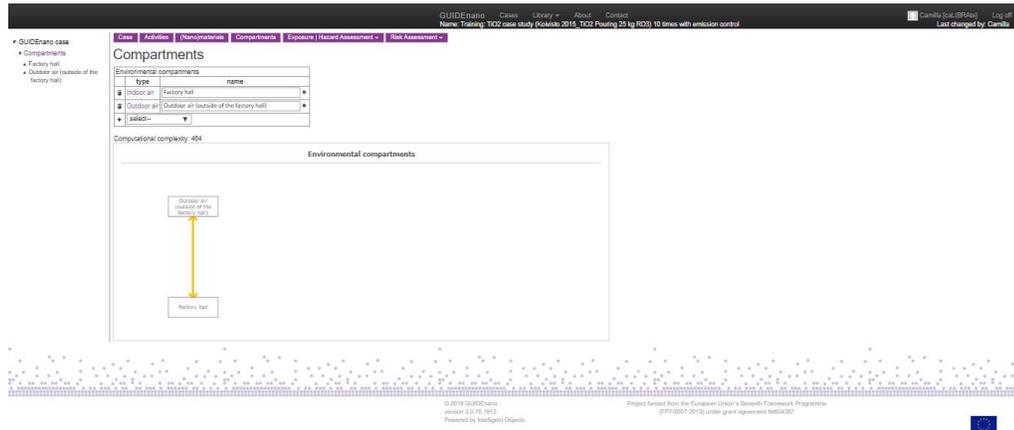
Present at:
Pouring 25 kg RD3 10 times with emission control TiO2 nanomaterials that are poured during the activity
Pouring 25 kg RD3 10 times with emission control TiO2 contained in the formulated paint
Pouring 25 kg RD3 10 times with emission control Emitted particles into the room (indoor)

At the bottom of the page, there is a footer with the following information: '© 2019 GUIDEnano version 3.0.70.1912 Powered by Intelligent Objects', 'Project funded from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement N656387', and the European Union flag.



Compartment framework

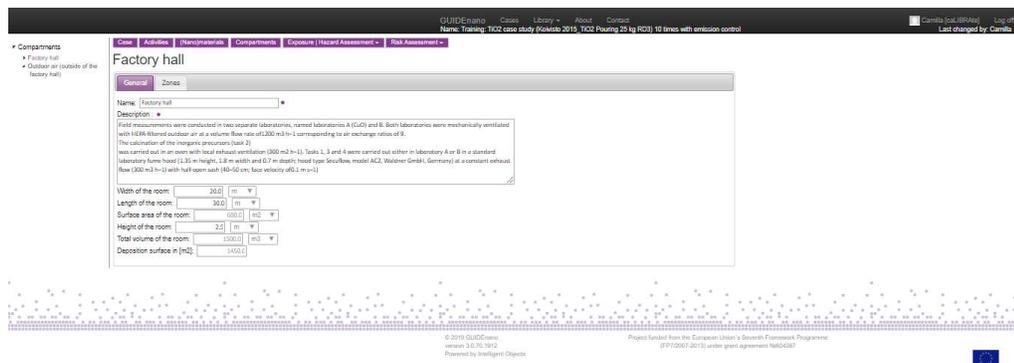
This framework is used to describe in which “system” or “environmental compartments” the released materials will first enter before getting in contact with the exposed species.



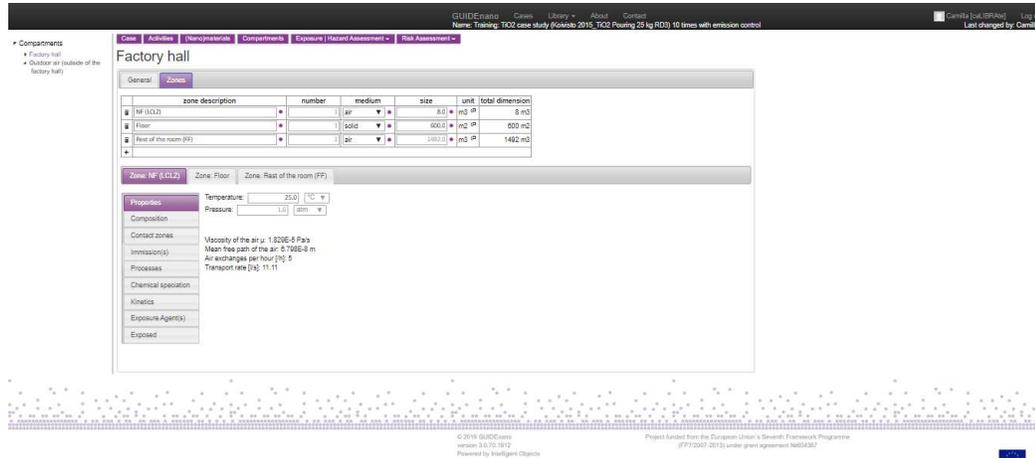
There are two groups of compartment type: the system compartment (which are manmade like as sewage system, waste water treatment plant, indoor air (room) and landfill site) and the environmental compartment (fresh water, estuarine, marine, fresh water sediment, salt water sediment, outdoor air and soil).

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

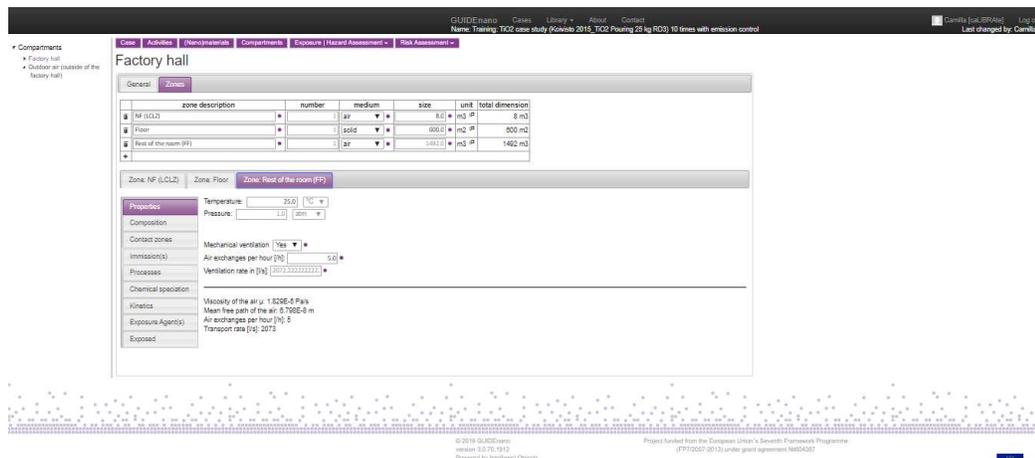
General information: for each compartment there are specific properties to fill. For example, in this case 2 compartments are defined, outdoor air and (Factory (indoor air)). For the compartment Factory Hall (indoor air), the user must enter a compartment name and a description and the room dimension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



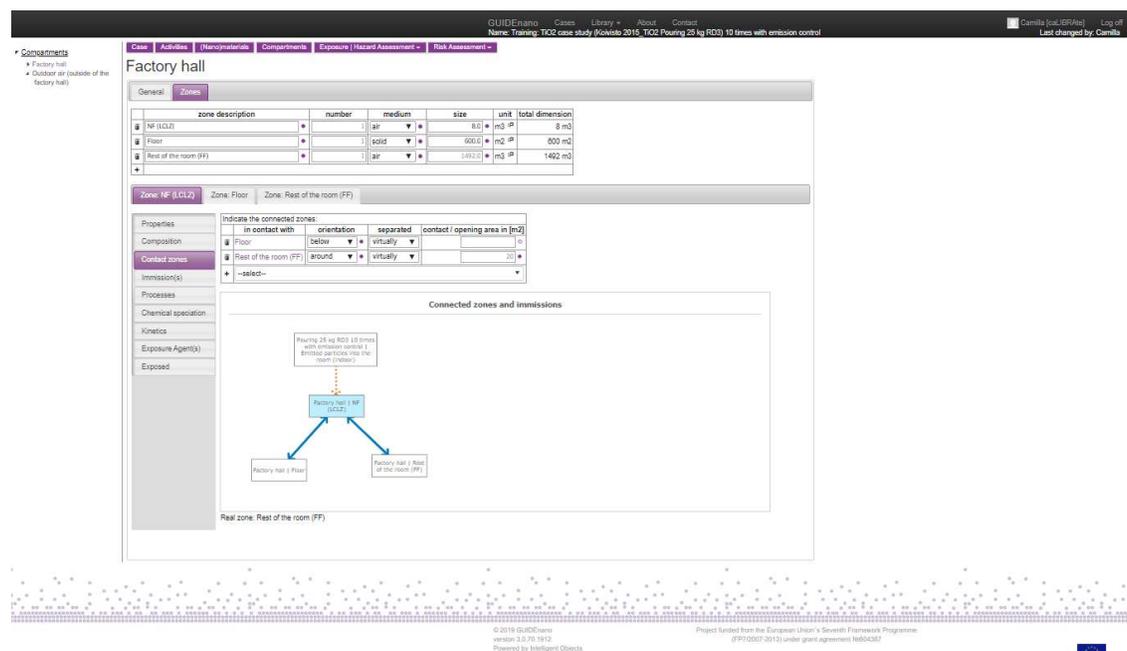
Zones: defines the different zones within the compartment. In this case, 2 compartments were defined, outdoor air and Factory (indoor air).



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”.



Factory hall

zone description	number	medium	size	unit	total dimension
NF (LCLZ)	1	air	8.6	m ³	8 m ³
Floor	1	solid	600.0	m ²	600 m ²
Rest of the room (FF)	1	air	1492.0	m ³	1492 m ³

Zone: NF (LCLZ) | Zone: Floor | Zone: Rest of the room (FF)

Indicate the connected zones:

in contact with	orientation	separated	contact / opening area in [m ²]
Floor	below	virtually	20
Rest of the room (FF)	around	virtually	

Connected zones and immissions

Diagram showing connections between zones: Factory hall | NF (LCLZ) is connected to Factory hall | Floor and Factory hall | Rest of the room (FF). A note indicates: "Pouring 25 kg RD3 10 zones with emission option 1. Emission air flows into the 'Rest of the room'."

Real zone: Rest of the room (FF)

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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.



GUIDEnano: Cases Library Floor Contact
Name: Training: TIC2 case study (Kövalds 2015, TIC2 Flooring 25 kg RD3) 10 times with emission control
Camilla Loui-SPPAHL Log off
Last changed by Camilla

Compartment: Factory hall
Outdoor air (outside of the factory hall)

Case Activities Nanomaterials Compartments Exposure Hazard Assessment Risk Assessment

Factory hall

General Zones

zone description	number	medium	size	unit	total dimension
NF (LCL2)	1	air	8.2	m3 IP	8 m3
Floor	1	solid	600.2	m2 IP	600 m2
Rest of the room (FF)	1	air	1492.2	m3 IP	1492 m3

Zone: NF (LCL2) Zone: Floor Zone: Rest of the room (FF)

Properties: Select or add a new exposed human population or eco species
 Composition: Workers 1 exposure NF (LCL2)
 Contact zones: --select--
 Immission(s)
 Processes
 Chemical speciation
 Kinetics
 Exposure Agent(s)
 Exposed

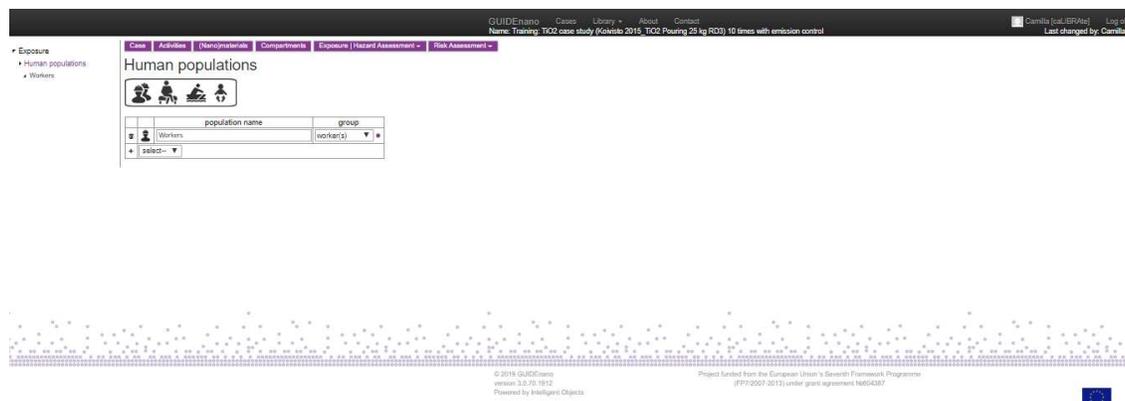
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 Project funded from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement N6864387

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.

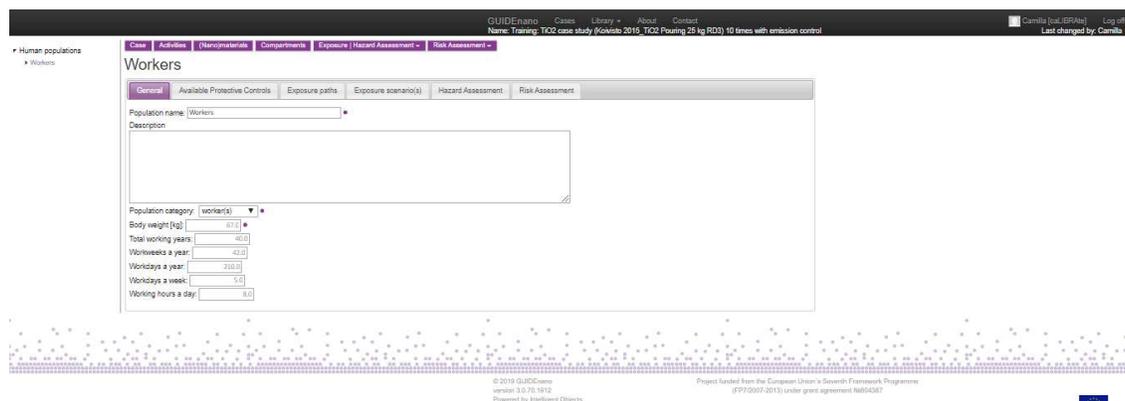


Exposure framework and Hazard assessment framework

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.).



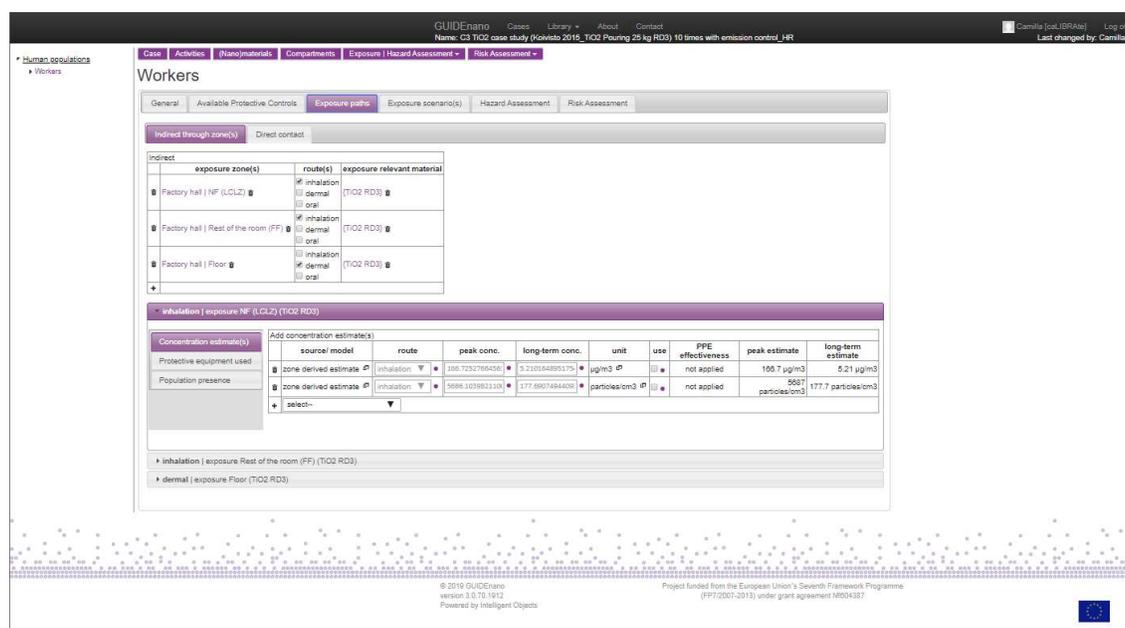
Moreover, body weight and information about working frequency can be provided, otherwise default values are used.

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



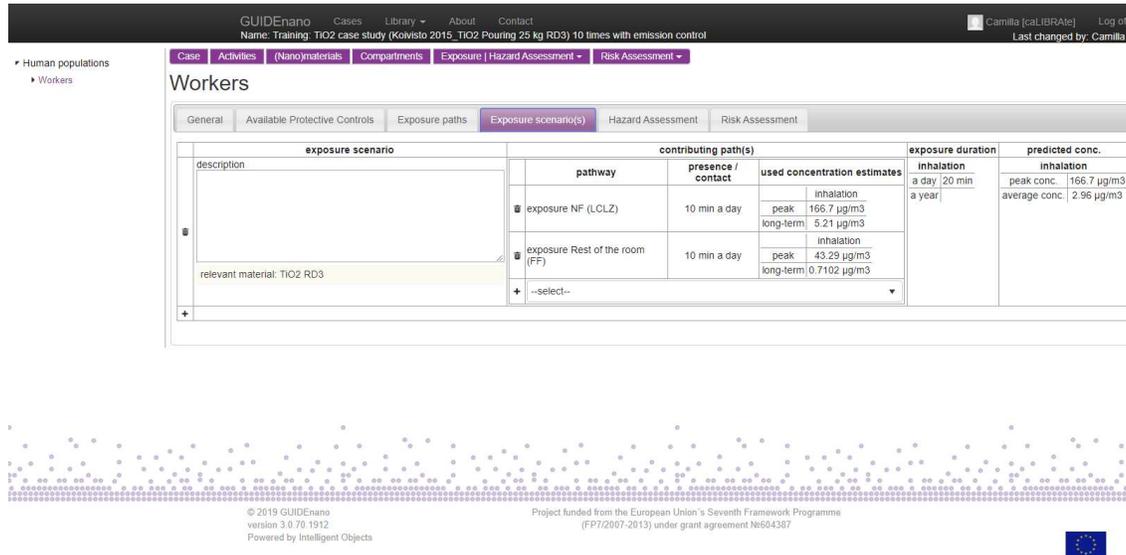
Hazard assessment tab, the Population presence need to be filled for the exposure path(s) previously defined, depending on the presence of the worker in the zones. In this case, we assume that workers are present in NF and FF for 10 minutes each day, during 210 working days in 1 year. For this case we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

The screenshot shows the 'Workers' tab in the caLIBRAtE software. The 'Population presence' section is active, showing input fields for 'Total time to consider' (set to 210 days), 'Duration' (set to 10 min), and 'Period of presence in zone' (set to 10 min). The 'Presence per zone during a (working) day' section shows a 3D bar chart with a value of 210 days. The 'Presence per zone during a (working) year' section shows a 3D bar chart with a value of 210 days. The interface also includes a table for 'Exposure paths' and 'Exposure relevant hazards'.

This screenshot is identical to the one above, showing the 'Workers' tab in the caLIBRAtE software. The 'Population presence' section is active, showing input fields for 'Total time to consider' (set to 210 days), 'Duration' (set to 10 min), and 'Period of presence in zone' (set to 10 min). The 'Presence per zone during a (working) day' section shows a 3D bar chart with a value of 210 days. The 'Presence per zone during a (working) year' section shows a 3D bar chart with a value of 210 days. The interface also includes a table for 'Exposure paths' and 'Exposure relevant hazards'.

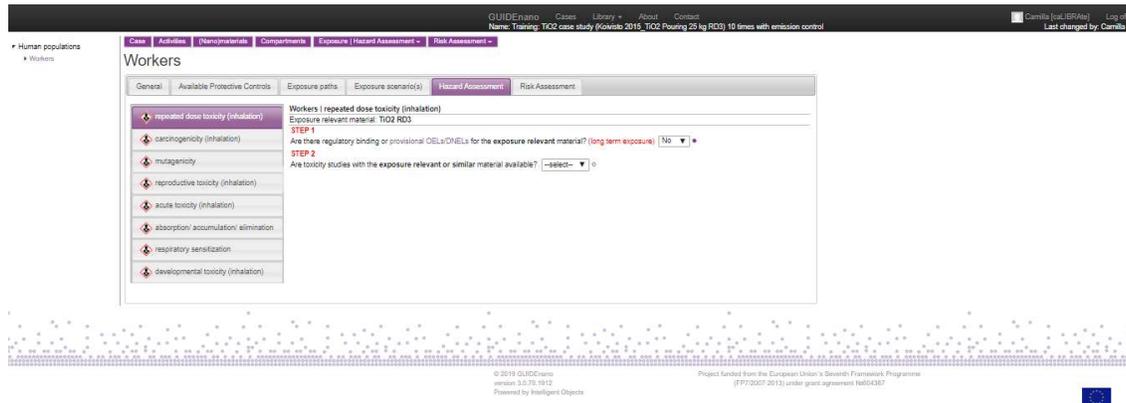


Exposure scenario(s): is generated by the user by clicking “+” and selecting the contributing path for the exposure. The Tool automatically report in the table the estimated concentration of the exposure relevant NM in the zones defined.



exposure scenario	contributing path(s)			exposure duration	predicted conc.
	pathway	presence / contact	used concentration estimates		
description relevant material: TiO2 RD3	exposure NF (LCLZ)	10 min a day	inhalation peak 166.7 µg/m3 long-term 5.21 µg/m3	inhalation a day (20 min a year)	inhalation peak conc. 166.7 µg/m3 average conc. 2.96 µg/m3
	exposure Rest of the room (FF)	10 min a day	inhalation peak 43.29 µg/m3 long-term 0.7102 µg/m3		

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,



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).

GUIDEnano Cases Library About Contact
Name: Training: TiO2 case study (Kowisto 2015, TiO2 Pouring 25 kg RD3) 10 times with emission control
Camilla (caLIBRAte) Log off
Last changed by: Camilla

Human populations
Workers

Case Activities (Nano)materials Compartments Exposure | Hazard Assessment - Risk Assessment -

Workers

General Available Protective Controls Exposure paths Exposure scenario(s) Hazard Assessment Risk Assessment

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

Describe the safety limit value for the exposure relevant material:

Dose descriptor	critical dose	unit	duration	exposure relevant material	source / comment
OEL	6.0	mg/m ³	long-term	TiO2 RD3	Table 1 in the paper

STEP 4
Final safety limit value for this endpoint:

Type	Final safety limit value	Uncertainty
DNEL (long-term)	DNEL 6 mg/m ³	0.0x

Low Medium High
RCR

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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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Human populations
Workers

Case Activities (Nano)materials Compartments Exposure | Hazard Assessment - Risk Assessment -

Workers

General Available Protective Controls Exposure paths Exposure scenario(s) Hazard Assessment Risk Assessment

Human exposure
Workers

Hazard endpoints to assess

Scenario(s)	repeated dose toxicity		carcinogenicity		mutagenicity		reproductive toxicity		acute toxicity		absorption/accumulation/elimination	sensitization	irritation/corrosion	developmental toxicity
	inhalation	oral/dermal	inhalation	oral/dermal	inhalation	oral/dermal	inhalation	oral/dermal	inhalation	oral/dermal	respiratory/oral/skin	skin	inhalation	oral/dermal
Pouring of 25 kg of TiO2 RD3 10 times with emission control	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫	🚫

Risk characterization
Pouring of 25 kg of TiO2 RD3 10 times with emission control

RCR=1
Risk Characterization Ratio (RCR)
0.0001931

repeated dose toxicity (inhalation)
repeated dose toxicity (oral/dermal)
mutagenicity
reproductive toxicity (inhalation)
acute toxicity (inhalation)
absorption/accumulation/elimination
irritation/corrosion
developmental toxicity (inhalation)

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