

## Electronic Supplementary Information (ESI)

### Evaluating environmental risk assessment models for nanomaterials according to requirements along the product innovation Stage-Gate process

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**Table S1a.** Description of the overall nanomaterial environmental assessment model criteria and stakeholder response options pertaining to model features, applicability and resources needed to run the model.

OVERALL CRITERIA FOR RISK ASSESSMENT			
Model features, applicability and needed resources	Criteria	Description/example	Response options
	Maximal costs	What are the maximal costs running the model may infer, incl. time to fill in the model with all necessary parameters?	(in k€)
	Maximal duration	What is the maximal time running the model may take, incl. time to gather all necessary input parameters? Time in duration, not in spent hours.	(in days)
	Market-readiness of model (acceptance/validation stage of model)	What level of market-readiness and acceptance should the model have?	<u>Choose one from list:</u> Prototype, Market-ready, Peer-reviewed, Validated, Accepted by OECD, Other
	Availability/format of the model	Should the model preferably be web-based, for stand alone, part of internal system or other?	<u>Choose one from list:</u> Web-base Stand alone Part of internal system Not important Other
	Availability of guidance	How important is availability of updated guidance provided along with the model?	Rate from 0 (not important) to 5 (essential)
	Level of expertise needed to run the model	Expertise within chemistry	<u>Choose one from list:</u> None Low Medium High Specialist Other
		Expertise within toxicology/ecotoxicology	
		Expertise within human exposure/environmental exposure and fate science	
	Combined human and environmental risk assessment	Should the model address both human and environmental risk?	Yes/No
	Transparency	How important is the model transparency for decisions and calculations?	Rate from 0 (not important) to 5 (essential)
	Quality assessment/rating of input data included	Should the model include a quality assessment and rating of the input data?	Yes/No

**Table S1a** continued

OVERALL CRITERIA FOR RISK ASSESSMENT			
Model features, applicability and needed resources	Criteria	Description/example	Response options
	Precautionary considerations	How does the model preferably deal with data gaps?	<u>Choose one from list:</u> Model stops Default value used Estimated value used Other
	Iteration/adaptation possibilities	How important is the possibility of adding/changing data as it becomes available, or in a following stage?	Rate from 0 (not important) to 5 (essential)
	Product life cycle perspectives	Which parts of life cycle should the model include?	<u>Tick off one or more:</u> Synthesis Production Transport Use End-of-life
	Specificity to industry	Does the model need to be specific to certain industry type(s)?	Yes/No
	Availability of default values and scenarios	Should the model have the option to use default values and default scenarios when certain input is not available?	Yes/No
	Standardized terminology	How important is the use of standardized terminology?	Rate from 0 (not important) to 5 (essential)
	Number and complexity of input parameters	Should the model include few and simple input parameters or many and more complex parameters?	Rate from 0 (few and simple input parameters) to 5 (detailed and highly complex)
	Applicability for various NMs and product types	Is it important for the model to accommodate different NMs and product types (e.g. liquids, solids, coatings)?	Yes/No
	Possibility of comparing NMs with bulk	Is it important for the model to consider risk of NM compared to the bulk form of the material?	Yes/No

**Table S1b** Description of the nanomaterial environmental assessment model criteria and stakeholder response options pertaining to model output for hazard assessment.

OUTPUT REQUIREMENTS FOR ENVIRONMENTAL RISK ASSESSMENT			
Hazard assessment	Criteria	Description/example	Response options
	Hazard score/estimate	What type of hazard score/estimate is needed for decision making, if any?	<u>Choose one from list:</u> None Qualitative Quantitative
	CLP Classification for environmental effects	How important is assignment of CLP classification (according to the European Parliament and Council, 2008) for the NM or product?	Rank from 0 (not important) to 5 (essential)
	PBT/vPvB classification	How important is assignment of PBT/vPvB classification for the NM?	Rank from 0 (not important) to 5 (essential)
	Compliance with current or near future regulation	How important is the reporting of hazard output in accordance with regulations, e.g. ENM definition?	Rank from 0 (not important) to 5 (essential)
	Hazard specified for environmental compartments	For which environmental compartments should hazard be considered?	<u>Tick off one or more:</u> No specification necessary Freshwater Marine water Sediment Soil Sewage treatment plant
	Specification of acute and chronic hazards	How important is the reporting of hazard output specific to acute vs chronic effects?	Rank from 0 (not important) to 5 (essential)
	Specification for different biological species	How important is the reporting of hazard output specific to different biological species?	Rank from 0 (not important) to 5 (essential)
	Predicted no effect concentrations (PNECs)	Which type of data for PNEC estimation do you consider sufficient?	<u>Choose one from list:</u> Laboratory test Read-across Modelling (QSAR)
		For which environmental compartments are PNECs needed, if any?	<u>Choose one from list:</u> All Freshwater Marine water Sediment Soil Sewage treatment plant

**Table S1c** Description of the nanomaterial environmental assessment model criteria and stakeholder response options pertaining to model output for exposure assessment.

OUTPUT REQUIREMENTS FOR ENVIRONMENTAL RISK ASSESSMENT			
Exposure assessment	Criteria	Description/example	Response options
	Exposure score/estimate	What type of exposure estimate is needed for decision making, if any?	<u>Choose one from list:</u> None Qualitative Quantitative
	Combined exposures	Which combined exposure scenarios must be considered (if any)?	<u>Choose one from list:</u> Multiple production processes Multiple product applications Multiple life cycle stages All
	Unintentional exposure	Should unintentional release/exposure be included?	Yes/No
	Compliance with current or near future regulation	How important is the reporting of exposure output in accordance with regulations, e.g. ENM definition?	Rank from 0 (not important) to 5 (essential)
	Spatial scale considered	For which scale should the exposure be considered?	<u>Choose one from list:</u> Local National Regional Global All
	Temporal scale considered	How important is considerations of temporal dynamics/time-dependency?	Rank from 0 (not important) to 5 (essential)
	Exposure specified for environmental compartments	For which environmental compartments should exposure be considered?	<u>Tick off one or more:</u> No specification necessary Freshwater Marine water Sediment Soil Sewage treatment plant Air
	Predicted environmental concentrations (PECs)	Which type of data for PEC estimation do you consider sufficient?	<u>Choose one from list:</u> Modelling Monitoring Laboratory measurements Extrapolation Read-across
		For which environmental compartments are PECs needed (if any)?	<u>Choose one from list:</u> None All Freshwater Marine water Sediment Soil Sewage treatment plant Air
		Which units should the PECs be given in?	<u>Choose one from list:</u> mg/L No of particle/m <sup>3</sup> µg/cm <sup>3</sup>

**Table S1d** Description of the nanomaterial environmental assessment model criteria and stakeholder response options pertaining to model output for risk assessment.

OUTPUT REQUIREMENTS FOR ENVIRONMENTAL RISK ASSESSMENT			
Risk assessment	Criteria	Description/example	Response options
	Risk indicator type	What kind of risk indicator should the model provide?	<u>Choose one from list:</u> A numerical value (risk characterization ratio) A risk classification (low, medium, high) As "Risk/no risk"
	Value of risk estimate	Should the risk estimate be indicative, scientifically sound, or compliant with regulations?	<u>Choose one from list:</u> Indicative Scientifically sound Compliant with regulations
	Risk estimate approach	Which approach should the model output be based on?	<u>Choose one from list:</u> Banding Grouping Worst case estimation Semi-worst case estimation Realistic
	Uncertainty characterization of risk estimate	What uncertainty characterization should the model give, to have a sufficient impression of the uncertainty in the outcome for decision making at the next "gate"?	<u>Choose one from list:</u> None Qualitative Quantitative
	Quantitative uncertainty analysis of input parameters provided	How important is a provided quantitative uncertainty analysis for input parameters (showing where risk assessment is best refined in further stages)	Rank from 0 (not important) to 5 (essential)
	Risk specified for environmental compartments	For which environmental compartments should risk be considered?	<u>Tick off one or more:</u> No specification necessary Freshwater Marine water Sediment Soil Sewage treatment plant
	Advice on risk management	The importance of risk management advice provided by the model	Rank from 0 (not important) to 5 (essential)

**Table S2.** Full list of assessment criteria and response categories for nanomaterial environmental assessment models.

Assessment criteria	Description of criteria	Response categories
Time/cost to parameterise model	What are the maximal costs to calculate and input all of required parameters into the model?	Minutes-Hours, Hours-Day, Days-Weeks, Weeks-Months
Level of expertise	What level of expertise is needed by the user running the model, can it only be operated by experts or is the structure and guidance of sufficient quality that a non-expert would be able to use the tool with minimal training?	Novice, Intermediate, Expert
Time/cost to run model	What is the maximal time running the model may take, including the iterative process or running the model and updating input parameters to gain the desired result?	Minutes-Hours, Hours-Day, Days-Weeks, Week-Months
Approval status	What is the scientific and regulatory approval status of the model, has it been peer reviewed, is it widely used and accepted in the scientific community, has it been the subject of standardisation and/or regulatory approval?	Standardised, Peer reviewed, In development
Format	What is the format of the model, is it available in a stand-alone format, is it a web based tool or does it have another non-software format?	Online, Stand alone, Not software
Guidance available	Is there guidance on how to parameterise and operate the model available for potential users?	Yes, No
Combined Human and Environmental Risk Assessment	Does the model allow the user to assess both human and environmental risk or is the model designed for environmental risk assessment only?	Human & Environment, Environment Only
Transparency	What is the access status of the model? Is the model and the code published and available (free or at cost), is the code held by an owner who will allow access to the model or is the code help and not available for other users?	Code freely available, Code available on request, Code not available
Deterministic versus Probabilistic	Does the model result in deterministic or probabilistic prediction of environmental fate and transport, uptake and accumulation, hazard and risk?	Deterministic, Probabilistic
Model assumptions	When assessing fate, hazard and risk, does the model make worst case assumption or is it designed to make realistic predictions based on the best available information?	Precautionary, Realistic
Applicable in multiple regulatory settings	How many different regulatory setting and jurisdiction can the model be used in, for example does it have limited geographical scope, is it limited to relatively few product applications, does it consider only certain release pathways?	Many, Some, Few, Single
Model flexibility for material types	Is the model applicable to a wide range of different nanomaterials or is it restricted to use in only a few different types?	High, Some, One only
Full or part life-cycle considered	Does the model assessment fate, hazard and exposure over the full life-cycle of the nanomaterial enabled product or is it use restricted to only certain phase of production, use and release?	Full, Part, N/A

**Table S2.** Continued

<b>Assessment criteria</b>	<b>Description of criteria</b>	<b>Response categories</b>
Default parameter values supplied	How many of the parameters that are used in the model are predetermined in the model and how many are available to be modified or input by the user?	Most (>80%), Some (30-80%), Few (1-20%), None, N/A
Model complexity	How complex is the structure of the model, is it based on simple algorithms or a more integrated overall structure and design?	Advanced, Intermediate, Simple
Product specific	Is the model only usable for assessment with some types of product or can it be used with a wide range of different products and applications?	Yes, No
Can compare NMs to bulk chemicals	Does the model include a comparison of the fate, hazard and risk of nanomaterials with "bulk" materials of a similar type?	Yes, No
Includes nano-specific input data	Does the model require the input of parameters that are unique to nanomaterials or are the properties included rated to generic chemical features and environmental properties?	Yes, No
Nano-specific factor required	How many nano-specific characteristics are needed for the successful parameterisation of the model?	>10, between 5-10, between 2-5, 1 only, None
Regulatory compliance	Is the model compliant with the specific requirement of developing regulatory management regimes for nanomaterials?	Yes, No
Spatially resolved by area	How does the model consider the spatial distribution of nanomaterial exposure, hazard and risk in the environment, it is considered from a general or local perspective?	Average concentration, Site Specific, N/A
Geographical scale	If the model does consider spatial distribution of exposure, hazard and risk at what scale is this considered?	Country, Region, Catchment, Meters/Point, Multiple, N/A
Temporal consideration	Is the model designed to consider changes in exposure, hazard and risk over time in a static or dynamic way?	Static, Dynamic, N/A
Requires product specific information	Does the model require the input of information that is specific to the product that the nanomaterial may be used in?	Yes, No, N/A
Requires application specific information	Does the model require the input of information that is specific to the application that the nanomaterial may be used in?	Yes, No, N/A
Release estimates during use	Is information on the potential form and rate of release needed for modelling?	Yes, No, N/A
Predicts concentrations in Freshwater	Does the model output include a prediction of the concentrations that will be found in freshwater?	Yes, No, N/A
Predicts concentrations in Sediment	Does the model output include a prediction of the concentrations that will be found in sediment?	Yes, No, N/A

**Table S2.** Continued

<b>Assessment criteria</b>	<b>Description of criteria</b>	<b>Response categories</b>
Predicts concentrations in Air	Does the model output include a prediction of the concentrations that will be found in air?	Yes, No, N/A
Predicts concentrations in Soil	Does the model output include a prediction of the concentrations that will be found in soil?	Yes, No, N/A
Includes end of life assessment	Does the model include a component that assesses exposure, hazard and fate during the end of life of the nano-enabled product?	Yes, No, N/A
Type of hazard estimate	What is the nature of the estimate of hazard that arises from the use of the model?	Quantitative, Qualitative, N/A
Supports CLP classification	Does the model support a classification according to Classification, Labelling and Packaging criteria?	Yes, No, N/A
Supports PBT classification	Does the model support a classification according to Persistent, Bioaccumulative, Toxic criteria?	Yes, No, N/A
Type of hazard data used	What type of hazard information can be used in the model does it cover only in individual level response or can biomarker and ecological information be included?	All, Ecosystem functional, Acute, Chronic, In vitro/biomarker, N/A
Derives hazard estimate from	Are the estimates of hazard derived only from measured data or can modelled information be used?	Data, QSAR, Data & QSAR, N/A
Derives bioaccumulation factors	Does the model derive estimates of nanomaterial bioaccumulation factors?	Yes, No, N/A
Risk categorisation	What is in the nature of the assessment of risk, only yes/no or more quantitative?	Binary, Scaled, N/A
Accuracy of risk assessment	How is the risk represented and scaled?	Precise, Banded, Worst case, Estimation, N/A
Includes life-cycle perspective	Is the model designed so that different features of the product life cycle of the nanomaterial are explicitly considered?	Yes, No, N/A
Presents comparisons of PECs and PNECs	Does the model allow the comparison of predicted environmental concentrations with predicted no-effect concentrations?	Yes, No, N/A

**Table S3.** Full scoring scheme used to assess suitability of nanomaterial environmental assessment models according to each stakeholder criterion and innovation stage.

Criteria		Idea	Scope	Business case	R&D	Test & Validate	Launch	Monitor
Time/cost to parameterise model	Minutes-Hours	1	1	1	1	1	1	1
	Hours-Day	0.5	0.75	1	1	1	1	1
	Days-Weeks	0.25	0.25	0.5	0.5	1	1	1
	Week-Months	0.1	0.25	0.25	0.25	0.5	1	1
Level of expertise	Novice	1	1	1	1	0.75	1	1
	Intermediate	0	0.25	0.5	0.75	1	0.75	0.5
	Expert	0	0	0	0.5	0.75	0.5	0.25
Time/cost to run model	Minutes-Hours	1	1	1	1	1	1	1
	Hours-Day	0	0	1	1	1	1	1
	Days-Weeks	0	0	0	1	1	1	1
	Week-Months	0	0	0	0.5	0.5	0.5	0.5
Approval status	Standardised	1	1	1	1	1	1	1
	Peer reviewed	1	1	1	1	0	0	0
	In development	0.5	0.5	0.5	0	0	0	0
Format	Online	0	0	0	0	0	0.5	0.5
	Stand alone	1	1	1	1	1	1	1
	Not software	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Guidance available	Yes	1	1	1	1	1	1	1
	No	0.5	0	0	0	0	0	0
Combined Human and Env. Risk Assessment	Human & Environment	1	1	1	1	1	0.5	0.5
	Environment Only	1	1	1	1	1	1	1
Transparency	Code freely available	1	1	1	1	1	1	1
	Code available on request	0	0	0.5	0.5	0.5	0.5	0.5
	Code not available	0	0	0	0	0	0	0
Deterministic vs. Probabilistic	Deterministic	1	1	1	1	1	0.5	0
	Probabilistic	0	0	0.5	1	1	1	1
Model assumptions	Precautionary	1	1	1	0	0	0	0
	Realistic	0.5	0.5	0.5	1	1	1	1
Applicable in multiple regulatory settings	Many	1	1	1	1	1	1	1
	Some	0	0	1	1	1	1	1
	Few	0	0	0	1	1	1	1
	Single	0	0	0	1	1	1	1
Model flexibility for material types	High	1	1	1	1	1	0.5	0.5
	Some	0.5	0.5	0.5	1	1	0.5	0.5
	One only	0	0	0	1	1	1	1
Full or part life-cycle considered	Full	1	1	1	1	1	1	1
	Part	1	1	1	0	0	0	0
	N/A	0	0	0	0	0	0	0

**Table S3.** Continued

Criteria		Idea	Scope	Business case	R&D	Test & Validate	Launch	Monitor
Default parameter values supplied	Most (>80%)	1	1	1	1	0.5	0.5	0.5
	Some (30-80%)	0	0	0.5	0.5	1	1	1
	Few (1-20%)	0	0	0	0.5	0.5	1	1
	None	0	0	0	0.5	0.5	1	1
	N/A	0	0	0	0	0	0	0
Model complexity	Advanced	0	0	0	1	1	1	1
	Intermediate	0	0	1	1	1	1	1
	Simple	1	1	1	0	0	0	0
Product specific	Yes	0	0	1	1	1	1	1
	No	1	1	1	0	0	0	0
Can compare NMs to bulk chemicals	Yes	0.5	0	0.5	1	1	0.5	0.5
	No	0.5	0	0.5	0.5	0.5	0.5	0.5
Includes nano-specific input data	Yes	0	0	0.5	1	1	0.5	0.5
	No	1	1	1	0.5	0.5	0	0
Nano-specific factor required	>10	0	0	0	0	0.5	1	1
	between 5-10	0	0	0	0	0.5	1	1
	between 2-5	0	0	0	0.5	1	1	1
	1 only	0.5	0.5	1	1	1	0.5	0.5
	None	0.5	0.5	0.5	0.5	0.5	0	0
Regulatory compliance	Yes	1	1	1	1	1	1	1
	No	1	1	0	0	0	0	0
Spatially resolved by area	Average concentration	1	1	1	1	1	0.5	0.5
	Site Specific	0	0	0	0.5	0.5	0.5	1
	N/A	0	0	0	0	0	0	0
Geographical scale	Country	1	1	1	1	1	1	1
	Region	1	1	1	1	1	1	1
	Catchment	0	0	0	0	1	1	1
	Meters/Point	0	0	0	0	1	1	1
	Multiple	1	1	1	1	1	1	1
	N/A	0	0	0	0	0	0	0
Temporal consideration	Static	1	1	1	0	0	0	0
	Dynamic	0.5	0.5	0.5	1	1	1	1
	N/A	0	0	0	0	0	0	0
Requires product specific information	Yes	0.5	0.5	0.5	1	1	1	1
	No	1	1	1	0.5	0.5	0	0
	N/A	0	0	0	0	0	0	0
Requires application specific information	Yes	1	1	1	1	1	1	1
	No	1	1	1	1	0	0	0
	N/A	0	0	0	0	0	0	0

**Table S3.** Continued

Criteria		Idea	Scope	Business case	R&D	Test & Validate	Launch	Monitor
Release estimates during use	Yes	0	0	0	0.5	1	1	1
	No	1	1	1	0.5	0	0	0
	N/A	0	0	0	0	0	0	0
Predicts concentrations in Freshwater	Yes	0	0	1	1	1	1	1
	No	1	1	0	0	0	0	0
	N/A	0	0	0	0	0	0	0
Predicts concentrations in Sediment	Yes	0	0	0	0.5	1	1	1
	No	1	1	1	0.5	0	0	0
	N/A	0	0	0	0	0	0	0
Predicts concentrations in Air	Yes	0	0	0	0.5	1	1	1
	No	1	1	1	0.5	0	0	0
	N/A	0	0	0	0	0	0	0
Predicts concentrations in Soil	Yes	0	0	0	0.5	1	1	1
	No	1	1	1	0.5	0	0	0
	N/A	0	0	0	0	0	0	0
Includes end of life assessment	Yes	0.5	0.5	1	1	1	1	1
	No	0.5	0.5	0.5	0	0	0	0
	N/A	0	0	0	0	0	0	0
Type of hazard estimate	Quantitative	0	0	0	1	1	1	1
	Qualitative	1	1	1	0	0	0	0
	N/A	0	0	0	0	0	0	0
Supports CLP classification	Yes	0	0	1	1	1	1	1
	No	1	1	0.5	0.5	0	0	0
	N/A	0	0	0	0	0	0	0
Supports PBT classification	Yes	1	1	1	1	1	1	1
	No	1	1	0.5	0.5	0	0	0
	N/A	0	0	0	0	0	0	0
Type of hazard data used	All	0	0	0	1	1	1	1
	Ecosystem functional	1	1	1	1	1	1	1
	Acute	1	1	1	1	1	0.5	0
	Chronic	0	0	0	1	1	1	1
	In vitro/biomarker	1	1	1	1	0	0	0
	N/A	0	0	0	0	0	0	0
Derives hazard estimate from	Data	0	0	0	1	1	1	1
	QSAR	1	1	1	1	0	0	0
	Data & QSAR	1	1	1	1	1	1	1
	N/A	0	0	0	0	0	0	0
Derives bioaccumulation factors	Yes	1	1	1	1	1	1	1
	No	0	0	0	0	0	0	0
	N/A	0	0	0	0	0	0	0

**Table S3.** Continued

Criteria		Idea	Scope	Business case	R&D	Test & Validate	Launch	Monitor
Risk categorisation	Binary	1	1	1	0	0	0	0
	Scaled	0	0	0	1	1	1	1
	N/A	0	0	0	0	0	0	0
Accuracy of risk assessment	Precise	0	0	0	1	1	1	1
	Banded	1	1	1	1	1	0	0
	Worst case	1	1	1	0	0	0	0
	Estimation	1	1	1	0	0	0	0
	N/A	0	0	0	0	0	0	0
Includes life-cycle perspective	Yes	1	1	1	1	1	1	1
	No	1	1	1	0	0	0	0
	N/A	0	0	0	0	0	0	0
Presents comparisons of PECs and PNECs	Yes	0.75	0.75	1	1	1	1	1
	No	0.75	0.5	0.25	0.25	0.1	0.1	0.1
	N/A	0	0	0	0	0	0	0