

Unclassified**English - Or. English****30 March 2020****ENVIRONMENT DIRECTORATE
CHEMICALS COMMITTEE****Working Party on Manufactured Nanomaterials****Physical- chemical Decision Framework Worksheets****Annex to document ENV/JM/MONO(2019)12**

This is an accompanying document to the PHYSICAL-CHEMICAL DECISION FRAMEWORK TO INFORM DECISIONS FOR RISK ASSESSMENT OF MANUFACTURED NANOMATERIALS - Series on the Safety of Manufactured Nanomaterials No. 90 [ENV/JM/MONO(2019)12].

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Annex 1: Worksheets to facilitate the information gathering for the Physico-Chemical Decision Framework to Inform Decisions for Risk Assessment

This series of Worksheets is a companion document to the *Physico-Chemical Decision Framework to Inform Decisions for Risk Assessment*.¹ It is intended to help guide users during the substance identification and information gathering steps of the Decision Framework by providing an outline of relevant parameters for data collection and population.

The framework underlines the importance of integrating specific information needs (i.e. purposes) with physico-chemical properties measurements. As a whole, the framework is intended to clarify requirements and reduce uncertainty in the applicability of testing and measurements for resolving knowledge gaps. Apart from a fundamental base-set of physico-chemical parameters believed to be generally important, the framework does not impose a finite set of parameters and testing regimens. It is intentionally focused on the process of identifying and acquiring the most relevant physico-chemical parameters (and analysis considerations) for resolving perceived data gaps. Recognising the increasing complexity of emerging nanomaterials the use of grouping and read-across approaches are integrated in the process to ensure that the physico-chemical parameters identified remain both current and fit-for-purpose noting continuing advances in knowledge.

The Decision Framework consists of three primary evaluation phases identifying specific purposes and key physico-chemical parameters/endpoints for each purpose (Figure 1):

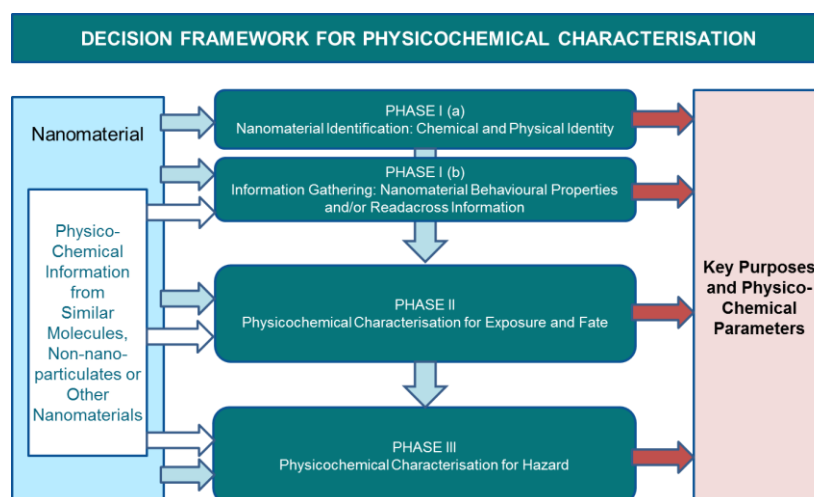
Phase I (a) Nanomaterial Identification (Worksheet 1a-c)

Phase I (b) Nanomaterial Information Gathering (Worksheets 2a-c, 3, 4, 5a-b, 6)

Phase II Human and Environmental Exposure and Fate Assessment (Worksheets 7.1a-c 7.2a-c)

Phase III Human and Environmental Hazard Assessment (Worksheets 8a-c and 9)

Figure 1: Overview of the Decision Framework for Physico-chemical Characterisation



¹ Series on the Safety of Manufactured Nanomaterials, No. 90. Physical-Chemical Decision Framework to Inform Decisions for Risk Assessment of Manufactured Nanomaterials. ENV/JM/MONO(2019)12

1. WORKSHEET 1a – General description of the material

| |
|--|
| GENERAL DESCRIPTION |
| Name and description of Product Form(s) (Dry Particle System or Particle System in Liquid) under consideration ² : |
| Description of Synthesis/Production Route: |
| Typical Storage Conditions: |

² In addition to ISO nomenclature standards (e.g., ISO/TS 80004-1:2015 (1) for core terms and ISO/TR 14786:2014 (2) for nomenclature considerations), Version 2.0 of the Uniform Description System for Materials on the Nanoscale (UDS) (3) could be considered in the context of these Worksheets. The UDS was developed in 2016, specific to nanomaterials, by the Committee on Data of the International Council for Science CODATA-VAMAS Working Group (WG) on Nanomaterials. This latest version contains 19 tables of detailed descriptors and their definitions that are directly applicable for reporting nanomaterials research results, identifying nanomaterials in regulations and standards, developing formats for nanoinformatics resources, specifying nanomaterials in commercial transactions, and other uses.

2. WORKSHEET 1b – Particle Chemical Identification

| CHEMICAL IDENTITY OF THE PARTICLE* (Chemical composition, molecular structure information, heterogeneity of the nanoparticle, and impurities) | | | | | | | | |
|---|-------------------|--------------------|-------------------------------------|-----------------|-------------------|--|--|--|
| CONSTITUENT SUBSTANCE IDENTITY (includes substance & impurities): | | | | | | CONSTITUENT STRUCTURE IDENTITY (measured or inferred): | | |
| Mass % | IUPAC name | Other names | Molecular structure/ formula | CAS name | CAS number | Location (Surface, subsurface, layer #, throughout, unknown) | Distribution (contiguous layer, discontinuous layer, random distribution, unknown, dispersant layer) | Determination method (synthesis procedure, EM & composition analysis...) |
| | | | | | | | | |
| | | | | | | | | |
| | | | | | | | | |
| | | | | | | | | |

Add additional rows as needed.

| CHEMICAL COMPOSITION AND MOLECULAR STRUCTURE OF NON-PARTICULATE CONSTITUENTS (e.g. dispersants) | | | | | | |
|--|-------------------|--------------------|-------------------------------------|-----------------|-------------------|---|
| Mass % | IUPAC name | Other names | Molecular structure/ formula | CAS name | CAS number | Purpose (e.g. dispersant, biocide) |
| | | | | | | |
| | | | | | | |
| | | | | | | |
| | | | | | | |

Add additional rows as needed.

* Attach details on measurements as available, including detailed description of sample preparation and methodology required (include rationale for selection of methods).

3. WORKSHEET 1c –Particle Physical Identity

| PARTICLE IDENTITY*: | |
|---|--|
| Particle Surface Area (as manufactured): | |
| Particle Density (skeletal, as manufactured): | |
| Particle Porosity (as manufactured, specific pore volume): | |
| Shape (as manufactured; 3D dimensions, aspect ratio, further description; add electron microscope micrograph): | |
| Crystallinity (as manufactured): | |
| Mean particle size (as manufactured): | |
| Attach characteristic micrograph (high resolution representative particle(s)) | Attach lower resolution micrograph (lower resolution field of particles) |
| Particle size distribution (image analysis or best practical dispersion, cumulative passing; % <100 nm by number) | Particle size distribution (best practical dispersion, cumulative passing; % <100 nm by number; % <100 nm by weight) |

* Attach details on measurements as available, including detailed description of sample preparation and methodology required (include rationale for selection of methods).

| Relevant particle system forms | |
|---------------------------------------|--------|
| Exists as a dry powder system? | Yes/No |
| Exists as particles in liquid? | Yes/No |
| Intended for aerosolisation? | Yes/No |

4. WORKSHEET 2a – Baseline Component Physico-Chemical Properties (Where available)

| | |
|---|--|
| PARTICLE IDENTITY*: | |
| For each component substance, as relevant: | |
| Physical state of the substance at 20 °C and 101.3 kPa: | |
| Melting/freezing point (major components and components with specific hazards): | |
| Boiling point (major components and components with specific hazards): | |
| Substance Density (particle component and liquid if relevant): | |
| Vapour Pressure (major components and components with specific hazards): | |
| Water solubility (particle component, as manufactured): | |

* Detailed description of sample preparation and methodology required (include rationale for selection of methods)

5. WORKSHEET 2b – Baseline Particle Physico-Chemical Properties (Where available)

| | |
|--|--|
| PARTICLE IDENTITY*: | |
| For the solid particle systems (at 20 °C and 101.3 kPa): | |
| Peclet number (as manufactured): | |
| Photocatalytic activity (as manufactured): | |
| Surface reactivity (as manufactured): | |
| Other unique/enhanced properties (as manufactured): | |
| Isoelectric point (as manufactured): | |
| pH of 1% suspension in deionised water (as manufactured): | |
| Dispersion stability at 1% in deionised water (as manufactured): | |
| Agglomeration/aggregation state (as manufactured): | |

* Detailed description of sample preparation and methodology required (include rationale for selection of methods)

6. WORKSHEET 2c – Potential Issues Of The Solid Particle System

| POTENTIAL ISSUES OF THE SOLID PARTICLE SYSTEM (Key to link to framework – Complete as possible) | | | |
|--|---|--------|------------------------------------|
| Shape | Is the substance or a component of the substance a WHO fibre? | Yes/No | If Yes, flag inhalation hazard |
| Reactivity | Is the substance engineered to promote reactivity? | Yes/No | If Yes, flag reactivity evaluation |
| Dispersal | Is the substance engineered to prevent agglomeration? | Yes/No | If Yes, flag migration evaluation |
| Known unique properties | Does the substance have known unique properties? | Yes/No | If Yes, flag unique properties |
| Known enhanced properties | Does the substance have known nano-enhanced properties? | Yes/No | Take note of enhanced properties |

7. WORKSHEET 3 – Considerations Due To Intended Use

| INTENTIONAL (UNIQUE) PROPERTIES ASSESSMENT (key- include where known) | | | |
|--|-----------------|--|--|
| | Property | Potential to modify exposure (human/environment)? | Potential to modify hazard (human/environment)? |
| What is the novel size dependent property? | | | |
| How does this property differentiate the materials from larger sized substances or alternative nanomaterials? | | | |
| Do other known nanoscale substances exhibit this property? If so, are identified implications known and related to physico-chemical parameters? | | | |
| What are the potential implications of this property in terms of human health? | | | |
| What are the potential implications of this property in terms of ecotoxicity? | | | |
| What are the potential implications of this property in terms of exposure (human/environment)? | | | |

| INTENDED USES AND REASONABLY ASCERTAINABLE USE INFORMATION | | | | | | | |
|---|---|--|--|--|--|---|--------------------------------|
| USE (including amount, e.g. tonnes per year) | Environmental conditions during use (e.g. pH, temperature) | Approximate percent mass content in end use | Physical state (solid matrix, powder, dispersion, paste, aerosol) | Potential human exposure route(s) | Potential environment exposure route(s) (including waste stage) | Particle transformation likely? If yes, fill Worksheets 5A & 5B (transformation) | Relevant notes/concerns |
| | | | | | | | |
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8. WORKSHEET 4 – Known Behaviour Identification Screening

| PHYSICAL HAZARDS IDENTIFIED FROM COMPONENT CHEMICAL SUBSTANCES | | |
|--|-------------------------------------|------------------------------|
| Hazard | Physical hazard related information | |
| | Substance(s) | Transformation anticipated?* |
| Explosive properties | | |
| Flammability | | |
| Autoignition temperature | | |
| Self-reactivity | | |
| Pyrophoricity | | |
| Water reactivity | | |

| HEALTH HAZARDS IDENTIFIED FROM COMPONENT CHEMICAL SUBSTANCES | | | | | |
|--|--------------------------------------|--|-----------------------------|-------|---------------------|
| Substance | Available hazard related information | | | | |
| | GHS hazard | Physical state of substance (ion, particle, etc.) | Exposure (as applicable) | route | Potency information |
| | | | | | |
| | | | | | |

| ENVIRONMENTAL IMPLICATIONS IDENTIFIED FROM COMPONENT CHEMICAL SUBSTANCES | | | | | |
|--|--------------------------------------|--|-----------------------------|-------|---------------------|
| Substance | Available hazard related information | | | | |
| | GHS hazard | Physical state of substance (ion, particle, etc.) | Exposure (as applicable) | route | Potency information |
| | | | | | |
| | | | | | |

| POTENTIAL PARTICLE BEHAVIOUR FORECAST ASSESSMENT* (Key to link to framework – Complete as possible) | | | |
|--|-----------------------------------|--------|--|
| /To estimate environmental compartment distribution | | | |
| Solubility in water | Solubility less than 100 mg/L? ** | Yes/No | If No, continue with std chemical substance evaluation |
| Dispersibility in water | | Yes/No | |
| Solubility in other relevant media | | Yes/No | |
| Dispersibility in other relevant media | | Yes/No | |
| Dissolution rate in water | | Yes/No | |
| Dissolution rate in other relevant media | | Yes/No | |
| Dustiness | | Yes/No | |
| Density | | | |
| Soil deposition potential | | | |
| Comments: | | | |

* Consider time scales for these processes where relevant.

** This is an arbitrary value that is not fixed yet. Also for the other parameters criteria need to be set to indicate what next steps may be.

9. WORKSHEET 5a – Initial Chemical Transformation Assessment

| Chemical transformations (consider all component substances and especially those that comprise the surface) | | | | |
|--|-----------|---------------------|------------------|---|
| Reaction with water? | Reaction: | Reaction half-life? | Form of products | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |
| Reaction with air? | Reaction: | Reaction half-life? | Form of products | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |
| Other relevant reactions within use matrix? | Reaction: | Reaction half-life? | Form of products | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |
| Relevant Photochemistry or Sensitive thermal reactions (e.g., free radical generation, decomposition) | Reaction: | Reaction half-life? | Form of Products | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |
| Other relevant reactions with environmental media? | Reaction: | Reaction half-life? | Form of products | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |

10. WORKSHEET 5b – Initial Physical Transformation Assessment

| Physical transformations | | | | |
|--|------------------------|--|---|---|
| Appreciable dissolution rate in water? | Equilibrium solubility | Dissolution half-life? (open system) | Impact of pH | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |
| Formation of irreversible aggregates (e.g. coalescence, mechanofusion)? | Mechanism of fusion | Conditions promoting fusion and timescale? | Is fusion intentional in application/use? | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |
| Other physical transformations | Mechanism | Timescale | Modifying factors | Time period after which 80% of the material is no longer nanoscale? |
| | | | | |

11. WORKSHEET 6 – Related Materials Screening – To identify relevant analogue particulate materials

Similar Composition (e.g. similar composition but different structure; similar composition but with or without certain chemical substances, surfaces, etc.)

| Substance | Relevant hazards | Related exposure considerations (including potential for co-exposures) | Key physico-chemical parameters identified for risk characterization | Notes: similarity/differences |
|-----------|------------------|--|--|-------------------------------|
| | | | | |
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Similar structural forms (e.g. similar structure different composition, similar coating layer different core-composition, physical, particle shape, etc.)

| Substance | Relevant hazards | Related exposure considerations (including potential for co-exposures) | Key physico-chemical parameters identified for risk characterization | Notes: similarity/differences |
|-----------|------------------|--|--|-------------------------------|
| | | | | |
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Related substances of similar use

| Substance | Relevant hazards | Related exposure considerations (including potential for co-exposures) | Key physico-chemical parameters identified for risk characterization | Notes: similarity/differences |
|-----------|------------------|--|--|-------------------------------|
| | | | | |
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12. WORKSHEET 7.1a – Exposure And Fate Assessment – Air

Considerations on Potential Exposure Routes

| DRY PARTICLE SYSTEMS | | |
|--|--|--|
| Key purposes: | Specific purposes: | Physico-chemical parameters and method considerations |
| Determine potential exposure routes of the material when aerosolised | Determine if exposure to human lungs and olifactory is significant: <ul style="list-style-type: none"> - Estimate concentration in air - Estimate inhalation exposure - Estimate transport through the lungs - Estimate accumulation site or clearance | Relevance of surrogate aerosolising method to real world exposure scenarios Relative impact of environmental conditions (e.g. humidity, electrostatics) |
| | Determine if oral exposure to human gastro-intestinal tract is significant <ul style="list-style-type: none"> - Estimate transport through the Intestinal tract - Affinity to Intestinal Mucosal layer - Properties influencing transcytosis (gap) | Propensity to agglomerate with aerosol concentration <ul style="list-style-type: none"> • Aerodynamic size distribution • Dustiness • Mass fraction inhalable • Mass fraction respirable • Shape and composition of respirable fraction • Shape and composition of inhalable fraction • Flexural rigidity of respirable and inhalable fraction • Surface properties to evaluate Clearance rate (e.g., phagocytosis, endocytosis) • Charge • Hydrophobicity • Surface properties |
| | Determine (roughly) potential dispersal to terrestrial ecosystem >> see Worksheet 7.1 B | |

13. WORKSHEET 7.1b – Exposure And Fate Assessment – Terrestrial Environment

Considerations on Potential Transformations in Terrestrial Environment

| DRY PARTICLE SYSTEMS | | |
|---|---|---|
| Key purposes: | Specific purposes: | Physico-chemical parameters and method considerations |
| Determine potential transformations that may occur in the terrestrial environment | Determine if chemical transformations are likely in a terrestrial environment | Relevant and characteristic chemical transformations along with relevant properties such as: <ul style="list-style-type: none"> • Water reactivity • Surface Passivation • Photo-transformations/degradation • Redox Reactions |
| | Determine if physical transformations are likely in a terrestrial environment | Relevant and characteristic physical transformation and relevant properties such as: <ul style="list-style-type: none"> • “irreversible” adhesion to other surfaces • Surface dissolution and reprecipitation (e.g. caking) • Solubility of reaction products above... etc. • Physical passivation of surfaces through adsorption • Changes in water dispersibility • Crystallinity |
| Estimate timescales and extent of transformations | Evaluate timescales and relevance of transformations | Reaction kinetics measurements |
| | Evaluate percent mass impacted and relevance for subsequent evaluation | Dissolution kinetics Accelerated weathering kinetics |
| | Identify relevant nanomaterial forms for consideration for hazard evaluations | Particle size analysis of transformed substance |

| DRY PARTICLE SYSTEMS | | |
|---|---|---|
| Key purposes: | Specific purposes: | Physico-chemical parameters and method considerations |
| Identify disposition and concern level in terrestrial environment | Compare / contrast with natural nanomaterials in environment | Contrast with natural nanomaterials <ul style="list-style-type: none"> • Composition • Crystallinity • Structure (surface/bulk) • Shape • Aggregation/agglomeration behaviour Propensity to deposit on other surfaces (surface affinity) Known unique properties Known enhanced properties |
| | Identify potential for migration through soil (typically low) | Soil deposition potential / heterocoagulation / filtration Known unique properties Known enhanced properties To be assigned: Soil sorption coefficient of dissolved components |

14. WORKSHEET 7.1c – Exposure And Fate Assessment – Aquatic Systems

Considerations on Potential Distribution to Aquatic Systems

| DRY PARTICLE SYSTEMS | | |
|--|---|--|
| Key purposes: | Specific purposes: | Physico-chemical parameters and method considerations |
| Determine potential exposure to and relevant form and compartmentalisation for aquatic environments: | Identify if the substance as a whole or in part is likely to dissolve? Identify if the substance is likely to agglomerate or heterocoagulate in aquatic media Determine likely compartment. | Representative aquatic media <ul style="list-style-type: none"> • Dissolution rate / Half-life • Equilibrium solubility • Interactions with naturally occurring ions and organic molecules Dispersibility in aquatic media <ul style="list-style-type: none"> • Designed dispersion mechanism (e.g. steric surface treatment) • Iso-electric point (IEP) of nanomaterial versus pH of aquatic media • Salinity of aquatic media (salting in / salting out) • Surface affinity / heterocoagulation • Hydrophobicity / hydrophilicity • Degradation rate Effective particle Péclet number Sedimentation kinetics Surface affinity / heterocoagulation |
| | Also consider: <ul style="list-style-type: none"> - Migration through soil into groundwater - Precipitation of dissolved components in water | |

| DRY PARTICLE SYSTEMS | | |
|--|---|--|
| Key purposes: | Specific purposes: | Physico-chemical parameters and method considerations |
| Evaluate concerns related to end-of-life disposition | For wastewater treatment: <ul style="list-style-type: none"> • Determine partitioning to sludge • Determine dissolution / degradation • Determine susceptibility to flocculation | <ul style="list-style-type: none"> • Sediment/soil disposition potential • Dissolution rate under relevant waste water treatment conditions • Degradation rate / chemical transformation rate under relevant waste water treatment conditions • Susceptibility to relevant flocculants • Dispersibility in wastewater • Surface affinity to activated sludge Known enhanced properties Known unique properties |

15. WORKSHEET 7.2a – Further Exposure And Fate Assessment Considerations

Considerations on Poorly Soluble or Immiscible Continuous Phase

| WET PARTICLE SYSTEMS | | |
|--|--|--|
| Key purposes | Specific purposes | Physico-chemical parameters and method considerations |
| Identify key issues transport and exposure issues for particles in wet systems where the liquid is not miscible or partly soluble with water | Determine environmental transport of liquid matrix | Solubility of liquid matrix Octanol-water partitioning coefficient (liquid) Effective liquid + particle system density Surface tension of liquid Viscosity of liquid / liquid + particle system Vapour pressure |
| | Determine if particle likely to separate from liquid phase | Spreading rate at aqueous interfaces / surface pressure kinetics Particle size distribution Dispersion stability Péclet number |
| Determine compartmentalisation in representative aquatic environments | Determine relevant timescale in water column | Representative aquatic media Dispersibility in aquatic media Sedimentation rate in aquatic media Particle Péclet number |
| | Determine relevant timescale in sediment | Representative sediment |
| | Determine migration potential in sediment | Sediment deposition potential (filtration/ surface affinity) |

16. WORKSHEET 7.2b – Further Exposure And Fate Assessment Considerations

Considerations on Potential Transformations in Aquatic Environment

| WET PARTICLE SYSTEMS | | |
|---|--|--|
| Key purposes | Specific purposes | Physico-chemical parameters and method considerations |
| Determine potential transformations that may occur in the aquatic environment | Determine if chemical transformations are likely in the representative aquatic environment (based on source material where applicable) | Relevant and characteristic chemical transformations and relevant properties such as: <ul style="list-style-type: none"> • Water reactivity • Surface passivation • Degradation • Redox reactions • Fouling / corrosion (e.g. sulphidisation) |
| | Determine if physical transformations are likely in the representative aquatic environment (based on source material where applicable) | Relevant and characteristic physical transformation and relevant properties such as: <ul style="list-style-type: none"> • “irreversible” adhesion to other surfaces • Dissolution rate in relevant media • Surface dissolution and reprecipitation (e.g. caking) • Solubility of reaction products above, etc. • Physical passivation of surfaces through adsorption • Changes in water dispersibility |
| Estimate timescales and extent of transformations in representative aquatic environment | Evaluate timescales and relevance of transformations (based on source material where applicable) | Reaction kinetics measurements Dissolution kinetics Accelerated weathering kinetics Particle size analysis of transformed substance |
| | Evaluate percent mass impacted and relevance for subsequent evaluation (based on source material where applicable) | |
| | Identify relevant nanomaterial forms for consideration for subsequent evaluations (based on source material where applicable) | |

17. WORKSHEET 7.2c – Further Exposure And Fate Assessment Considerations

Considerations on End-Of-Life Disposition

| WET PARTICLE SYSTEMS | | |
|--|--|--|
| Key purposes | Specific purposes | Physico-chemical parameters and method considerations |
| Evaluate concerns related to end-of-life disposition | For wastewater treatment: Determine partitioning to sludge Determine dissolution / degradation Determine susceptibility to flocculation | Sediment/soil disposition potential Dissolution rate under relevant waste water treatment conditions Degradation rate / chemical transformation rate under relevant waste water treatment conditions Susceptibility to relevant flocculants |

18. WORKSHEET 8a – Specific Hazard Considerations for Human Exposure - Dermal

| Key purposes | Specific purposes | Physico-chemical parameters and method considerations |
|--|--|--|
| Identify parameters that may modify dermal contact hazards | Determine factors that may enhance interactions with viable tissue <ul style="list-style-type: none"> - Chemical composition and impurities - Specific surface area - Particle size distribution - Shape - Surface chemistry - Charge / zeta potential - Free radical generation capacity - Dissolution rate - Agglomeration / aggregation - Crystallinity - Conduction band energy level - Corrosivity - | Relevant sweat or fluid media Biological pH range Particle size distribution Particle shape distribution Surface chemistry Crystallinity Dispersion and/or dissolution in sweat Surface affinity to epidermis / dermis Hydrophobicity Isoelectric point Surface reactivity Active agent release Chemical composition Specific surface area Unique properties Degradation rate Octanol-water partitioning of media soluble compounds (e.g. dispersant) pKa of soluble compounds |
| | Determine factors that may modify biological activity Determine factors that may modify kinetics / transport through the body, e.g.: <ul style="list-style-type: none"> - Dispersibility in plasma - Affinity to cell surfaces | |

19. WORKSHEET 8b – Specific Hazard Considerations for Human Exposure - Inhalation

| Key purposes | Specific purposes | Physico-chemical parameters and method considerations |
|---|---|---|
| Identify parameter that may modify pulmonary exposure hazards | Determine relevance of factors that may modify phagocytic clearance | Relevant pulmonary fluid, interstitial fluid, lysosomal fluid, or intracellular fluid |
| | Determine relevance of factors that may modify specific biological activity | Affinity to cell surfaces |
| | Estimate transport through the lungs | Factors that impact adsorption and adsorbed conformation of biomolecules: / pulmonary exposure hazard: |
| | Consider that response to initiating events from chemical (as opposed to simply particle) responses may result in changes in relevant fluid conditions and interactions | <ul style="list-style-type: none"> • Surface chemistry/defects • Surface energy • Crystallinity • Particle size • Particle shape • Isoelectric point • Stereochemical and coordination effects Surface reactivity Surface charge Conduction band energy Known unique properties Known enhanced properties Specific surface area Excluded Volume Free radical generation capacity Flexural rigidity Dispersibility in lung fluid & resulting Péclet number Surface affinity to lung tissue cells / surveillance cells Properties that modify phagocytosis clearance rate |

20. WORKSHEET 8c – Specific Hazard Considerations for Human Exposure – ORAL

| Key purposes | Specific purposes | Physico-chemical parameters and method considerations |
|---|--|--|
| Identify parameters that may modify oral exposure hazards | Determine potential transformations due to interactions with biological fluids | Relevant saliva, mucus, stomach, upper and lower intestinal fluids Relevant and characteristic chemical transformations and relevant properties such as: <ul style="list-style-type: none"> • Water reactivity • Surface passivation • Degradation • Redox reactions Relevant and characteristic physical transformation and relevant properties such as: <ul style="list-style-type: none"> • “irreversible” adhesion to other surfaces (e.g. fibre) • Surface dissolution and reprecipitation (e.g. caking) • Solubility of reaction products above... etc. • Physical passivation of surfaces through adsorption Dispersibility in fluid Surface affinity to other surfaces Unique properties Impact of progressive changes in media on transformations and dispersion |
| | Determine potential transformations upon ingestion | |
| | Estimate potential for transport into circulation See above | |

21. WORKSHEET 9 – Specific Hazard Considerations for the Environment

| | | |
|---|---|--|
| Identify parameters that may modify aquatic and sediment exposure hazards | Determine potential transformations due to interactions with test media | <p>Relevant and characteristic chemical transformations and relevant properties such as:</p> <ul style="list-style-type: none"> • Water reactivity • Surface passivation • Degradation • Redox reactions • Fouling /corrosion (e.g. sulphidisation) |
| | Determine agglomeration and dissolution rates | <p>Relevant and characteristic physical transformation and relevant properties such as:</p> <ul style="list-style-type: none"> • “Irreversible” adhesion to other surfaces • Dissolution and reprecipitation • Solubility of reaction products above, etc. • Physical passivation of surfaces through adsorption (e.g. NOM adsorption) |
| | Determine surface affinity to test organism | <ul style="list-style-type: none"> • Agglomeration rate • Dissolution rate • Surface chemistry • Surface energy • Isoelectric point / surface charge • Surface area • Shape • Péclet number <p>Known unique properties Known enhanced properties</p> |

Note that the relevance of specific physico-chemical parameters for behaviour in complex systems can be largely impacted by shape as well as chemical composition of the material and its surface. Hence using source materials and grouping to aid in narrowing physico-chemical parameter relevance is necessary and should overtime lead to more explicit rules for categories based on physico-chemical parameters for certain sets of materials.

22. References

- (1) ISO (2015). ISO/TS 80004-1:2015 - Nanotechnologies – Vocabulary – Part 1: Core terms. ISO report. International Organisation for Standardisation (ISO), Genève, Switzerland.
- (2) ISO (2014). ISO/TR 14786:2014 – Nanotechnologies -- Considerations for the development of chemical nomenclature for selected nano-objects. Technical Report. International Organization for Standardization (ISO). Available from: <https://www.iso.org/standard/55039.html>.
- (3) CODATA-VAMAS Working Group On the Description of Nanomaterials and Rumble J. (2016). Uniform Description System for Materials on the Nanoscale - Version 2.0. Report 56720. International Council for Science: Committee on Data for Science and Technology (CODATA) and Versailles Project on Advanced Materials and Standards (VAMAS). Available from: <https://zenodo.org/record/56720>.