Comparing pre-guideline literature data on dispersion stability for CeO_2 nanoparticles to current guideline requirements

Can we use literature data for concluding on the endpoint and grouping?

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Introduction

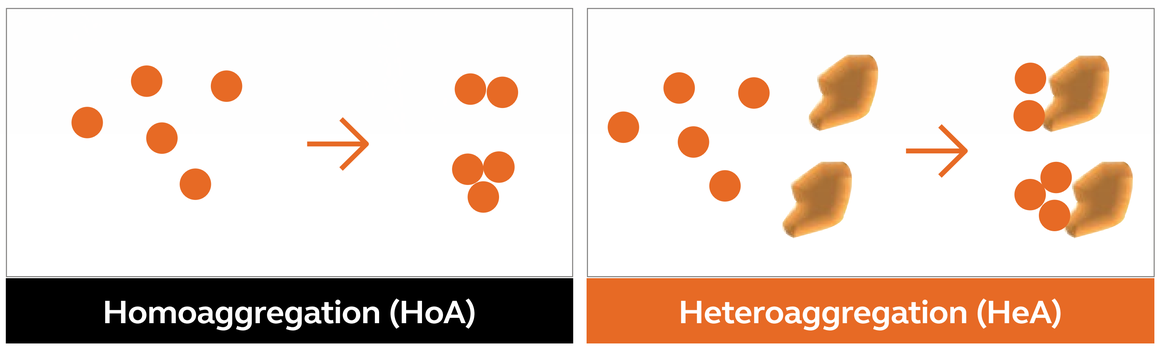
Dispersion stability depends on physicochemical characteristics of the nanoparticles and the suspension medium, as well as on the concentration of nanoparticles and other substances or particles in the medium. It is a mandatory endpoint for nanoparticles under EU REACH.

Two main processes can be distinguished: homoaggregation and heteroaggregation.

Following guidelines have been released so far to investigate these processes:

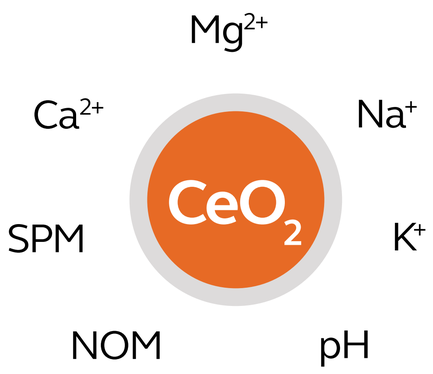
- OECD guideline 318 (2017) → Focus on homoaggregation
- OECD Series on Testing and Assessment No. 318 (2020/2021) → Suggest testing requirements for heteroaggregation

Most literature data on dispersion stability of CeO_2 nanoparticles are however pre-guideline studies. In this poster it is demonstrated that these data can however be used for covering the endpoint under EU REACH.



Guideline requirements

HoA	
Medium	Artificial, no suspended solids
Duration	6 h
NOM	0-10 mg DOC/L
pH	4-7-9
Ca^{2+}	0-1-10 mM
NP concentration	0.5-5E+12 particles/L
HeA	
SPM type	Mineral to natural
SPM concentration	To be calculated case by case



Investigated studies

Only uncoated spheroidal CeO_2 considered - as in EU REACH dossier.

	HoA (6 studies)	HeA (+HoA) (7 studies)
Medium	Artificial / natural / wastewater	
Duration	0 to 12 d	75 min – 12 mo
NOM	0-118 mg DOC/L	0.2-26 mg DOC/L
pH	3-11	4.6-10
Ca^{2+} *	0.1-30 mM	0.1-10 mM
NP concentration	2E+11-2E+16 particles/L	2E+10-8E+15
SPM type		Mineral / natural
SPM concentration		1.9-213 mg/L

* In most studies not only Ca^{2+} present, wide variety of ionic strength

Conditions covered with regard to suspension medium and particle concentration = broader than guideline/recommendations!

Main findings

- Increasing **natural organic matter (NOM)** concentration increases negative charge, therefore **increasing** electrostatic repulsion and **stability**.
- **Ionic strength (IS)** typically **reduces stability** by reducing electrostatic repulsion.
- The effect of pH is not always straightforward, however, **low pH can stimulate NOM adsorption**, therefore **adding to the prevention of aggregation**.
- **Increasing nanoparticle (NP) concentration reduces stability** (more collisions).
- **Increasing suspended matter (SPM)** concentration **reduces stability**, idem for concentration of 'depositional surfaces' in general.
- At **lower CeO_2 concentration** (< 1 mg/L), **heteroaggregation** is likely **dominant**, however, at higher concentrations, homoaggregation is likely dominant.
- **In general, fast removal (sedimentation)** is observed in waters where both hetero- and homoaggregation can take place. Removal rates varied between 99% within 1 day in a mesocosm study at 2.5 mg CeO_2/L and 80% within 12 days in natural water at 1 mg CeO_2/L.
- Nevertheless, **stable dispersions may occur under specific circumstances; typically high DOC in combination with low pH and low NP concentration** may result in longer removal rates. However, other combinations of medium composition and particle characteristics/ concentrations may also exceptionally lead to stable dispersions.
- Presence of **surfactants, oxidisers, complexing agents**, etc. which are sometimes added during processes (e.g., in polishing slurries to improve polishing performance), **may also lead to slower removal**, e.g., in wastewater derived from these processes.
- Above **conclusions are for uncoated CeO_2 nanoparticles**. Nanoparticles with surface functionalisation or coatings may behave differently.

Is guideline testing required to conclude on the endpoint?

- A **standardised way of testing** for both HoA and HeA may lead to **standardised comparison with other NPs** as well as derivation of constants (such as for attachment efficiency) which could be used in exposure models.
- For concluding on the EU REACH endpoint however, a **standardised test is not expected to bring additional insights.**

Implications for grouping?

- As the **current EU REACH dossier only covers spheroidal, uncoated, CeO_2 NPs**, and dissolution (no guideline data available either) has been observed to be minimal, **differences** between CeO_2 NPs covered in the dossier are **expected to be much more dependent on medium characteristics than on small differences in NP characteristics within this same set of nanoforms**.
- For **other shapes and surface functionalised or coated particles** however, **separate testing/evaluation** should be performed.