Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting information of the manuscript

Chronic dosing of a simulated pond ecosystem in indoor aquatic mesocosms: Fate and Transport of CeO_2 nanoparticles

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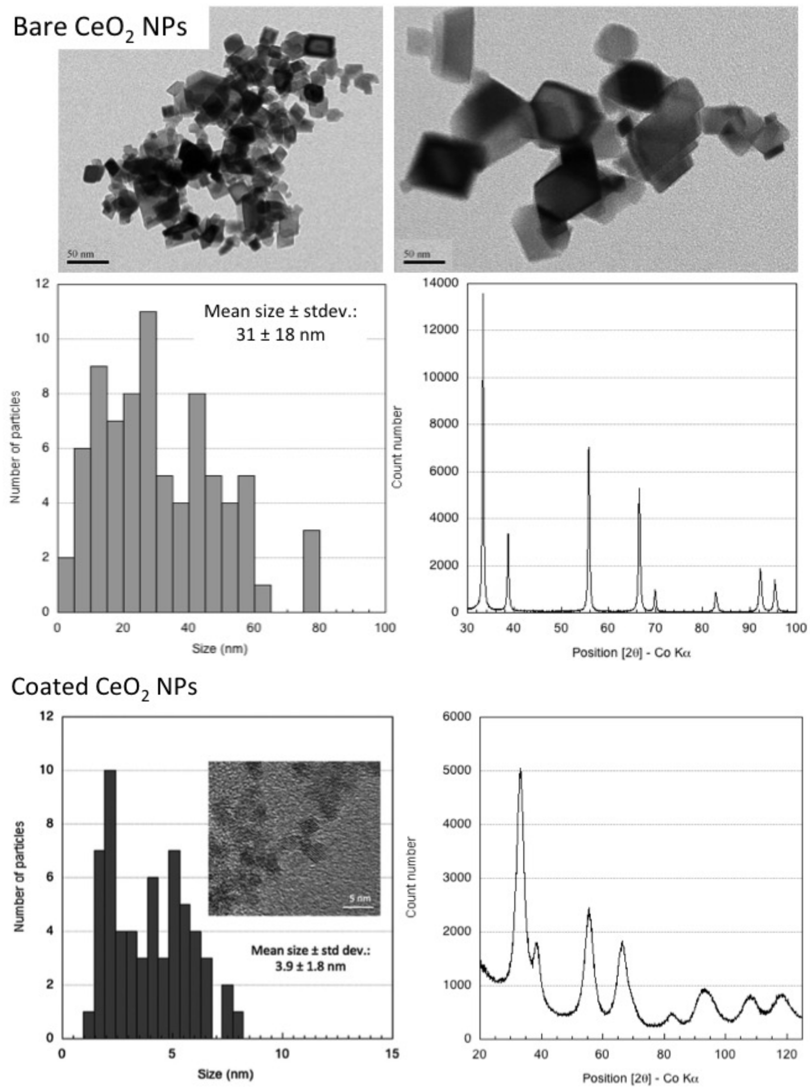


Figure S1. TEM images and X-ray diffractograms of bare CeO_2-NPs and coated CeO_2-NPs.

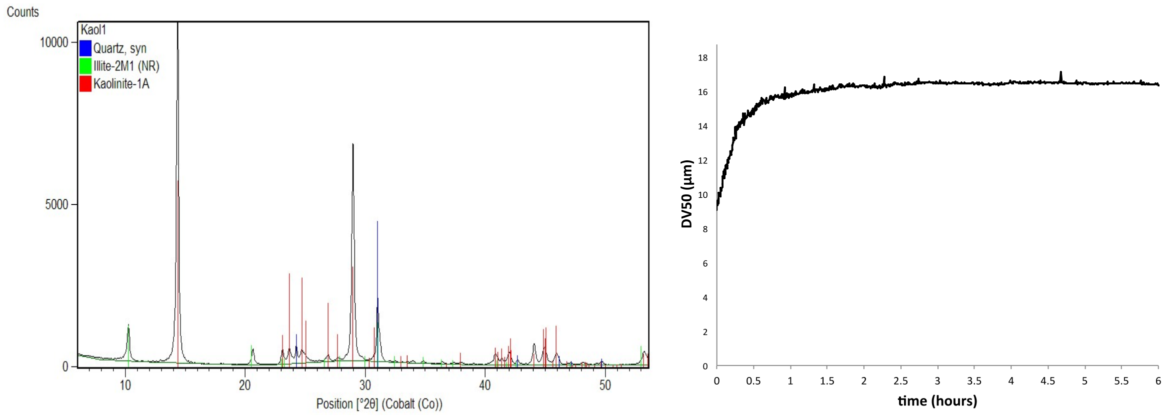


Figure S2. Characterization of the kaolinite particles used in the mesocosms. (left) X-ray diffractogram and (b) average hydrodynamic diameter (DV50) obtained using the Mastersizer 3000 (Malvern®).

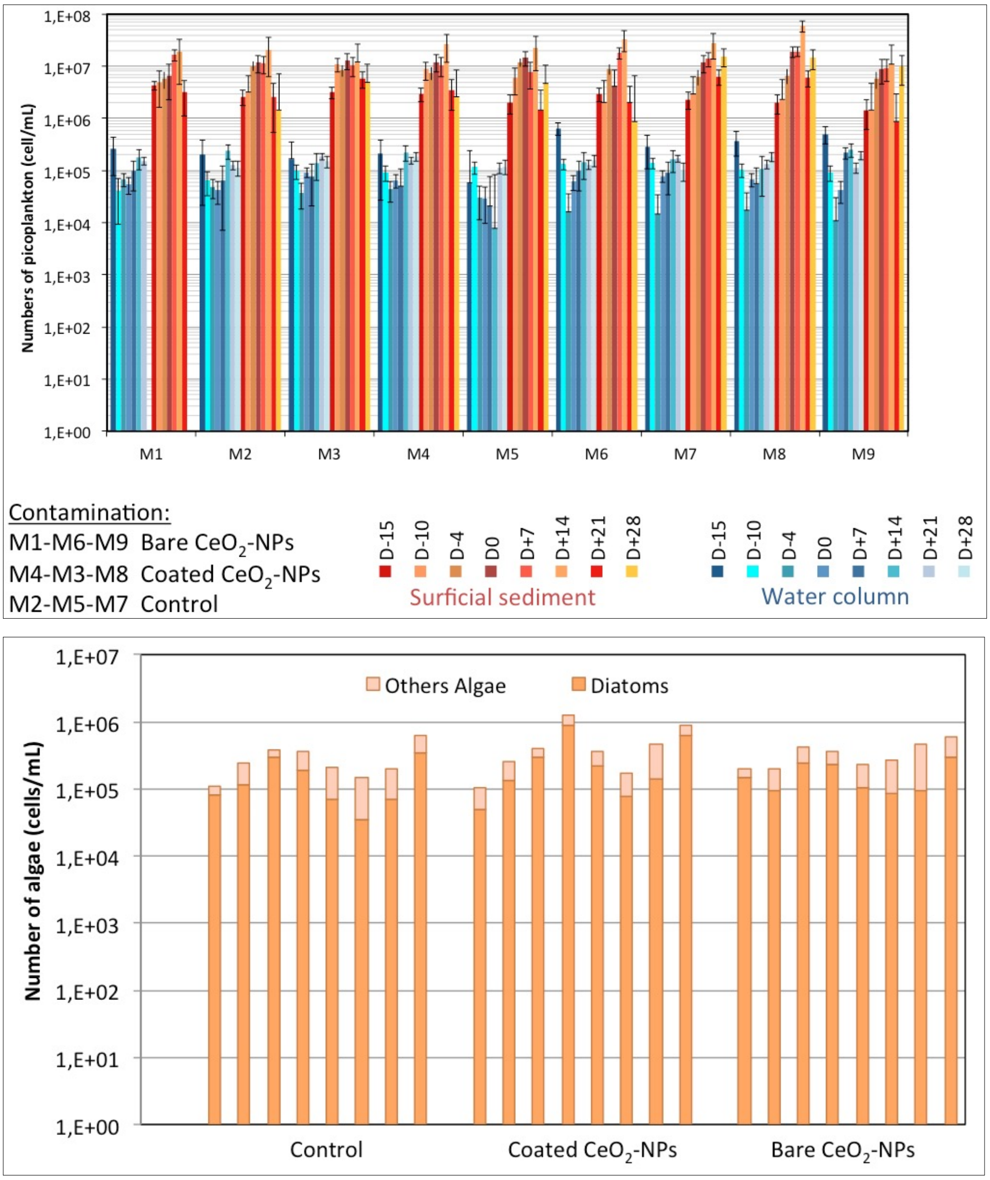


Figure S3. Number of picoplankton (in the water column and surficial sediments) and algae (in the surficial sediments) over time in the mesocosms.

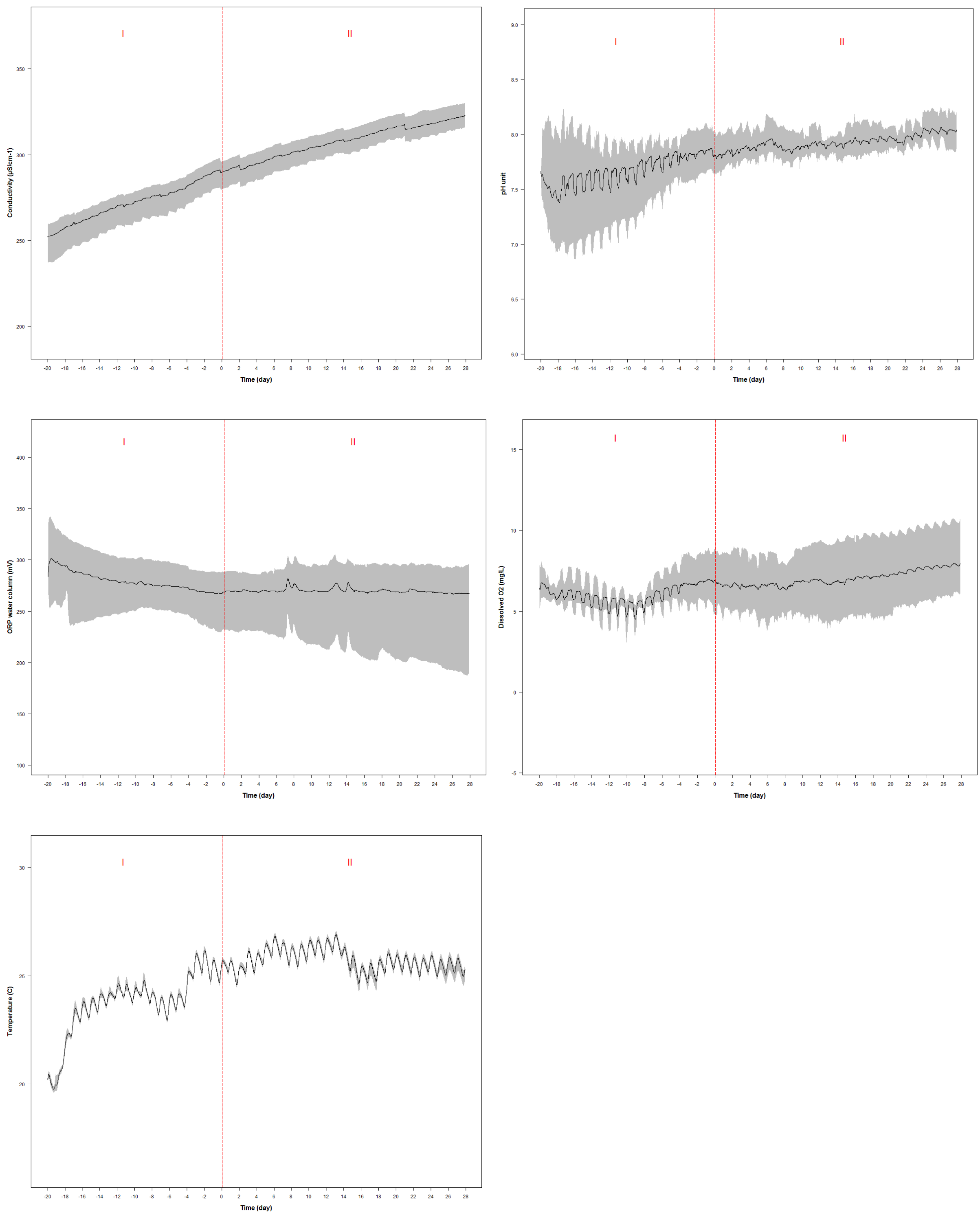
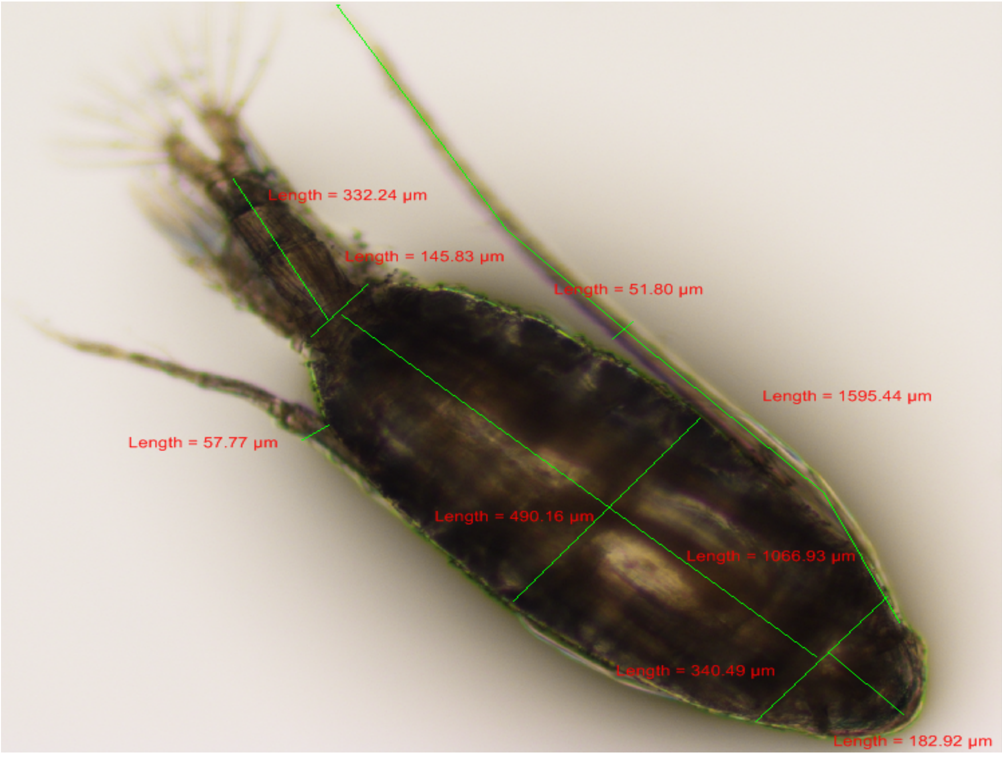


Figure S4. Evolution of the physico-chemical parameters in the water column of the mesocosms. Redox potential, dissolved oxygen, pH, and conductivity were measured during phases I (stabilisation) and II (contamination). Day 0 corresponds to the first dosing of NPs. The grey surface is defined by the maximum and minimum values of each parameter, and the dark line corresponds to the average values of the 9 mesocosms. One measurement was performed every 5 min.

Top view)



Side view)

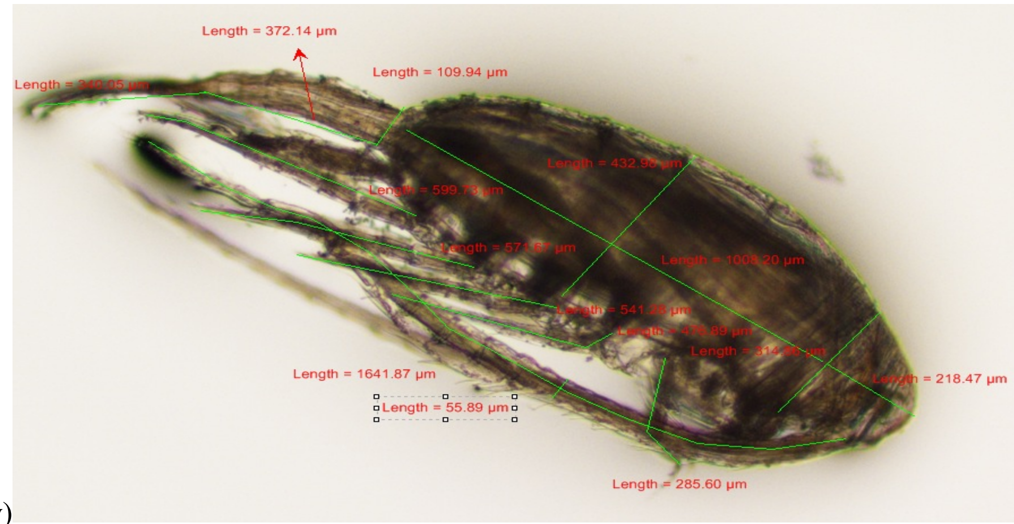


Figure S5. Estimation of biovolume of the *Eudiaptomus vulgaris* copepods introduced in the mesocosms. Copepods were divided into different geometrical sub-volumes. Cylinders for the body, antennas, legs and tail. Half-sphere for the head. Parameters for cylinders and half-spheres were measured on different profiles of the organism (using the side and top views). The cumulated volume of the antenna, legs and tail represent less than <6% of the total volume and were neglected for the calculations. The copepods sampled from the mesocosms have a biovolume of $2.6 \pm 0.5 \times 10^8$ µm^3 corresponding to $2.6 \pm 0.5 \times 10^4$ g considering a density of 1. Chemical results were expressed by kg of dried matter considering 80% of water in the organisms.

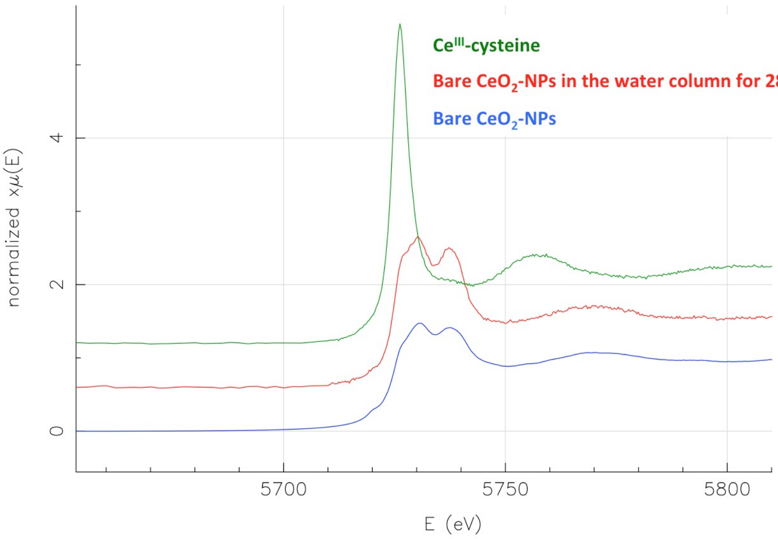


Figure S6. XANES spectra (Ce L_3-edge) of the ultracentrifuged-water column of the mesocosms exposed to bare CeO_2-NPs. Experimental spectra are compared to Ce^{III}-cysteine and initial NPs reference spectra.

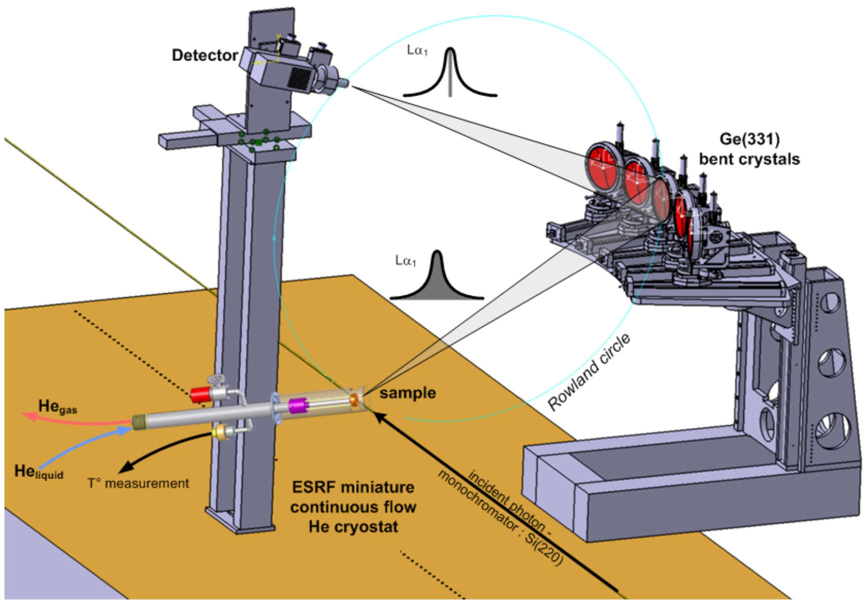


Figure S7. High energy resolution fluorescence detected x-ray absorption spectroscopy experimental set-up on CRG-FAME beamline (BM30b, ESRF, Grenoble, France). The five-crystal spectrometer was equipped with spherically bent Ge(331) crystals in a Rowland geometry. The spectrometer was aligned at 4.840 keV (Bragg angle: 80.72°) in order to select a fraction of the Ce-Lα1 fluorescence line. Crystals had a 1m radius of curvature and were provided by XRS TECH LLC company (Freehold, NJ, USA). The detector was a Silicon Drift Detector (energy resolution: 250 eV) in order to discriminate the fraction of the fluorescence signal diffracted by the crystals from the scattering ones and to improve the signal-to-noise ratio. A miniature small continuous flow helium cryostat from ESRF Sample Environment Support Service was used to cool down the samples and to protect them from radiation damages.

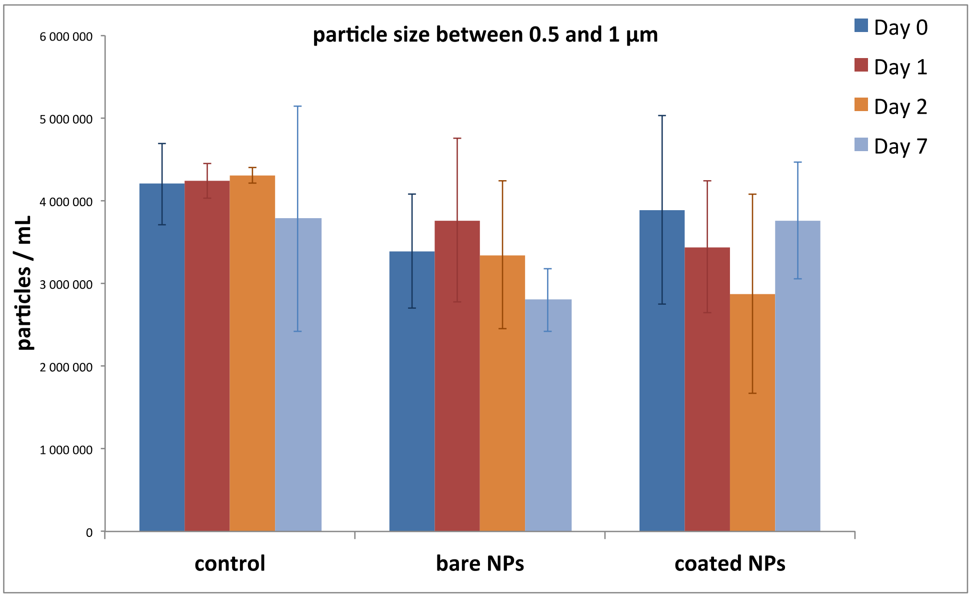


Figure S8. Number of suspended materials (size ranged between 0.5 and 1 µm) in the mesocosm water column as a function of the NPs injected (bare *versus* coated) during the first 7 days.

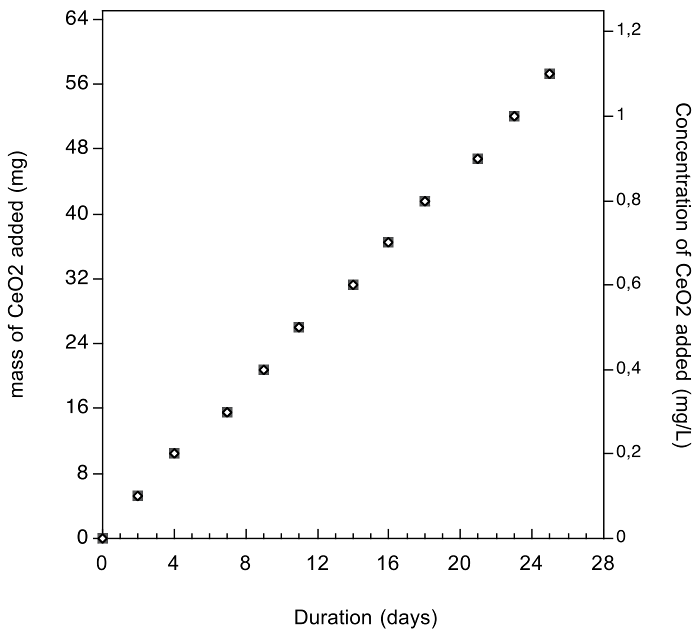


Figure S9. Dosing sequence of the water column of the mesocosms during the 28 days experiment.

Table S1. Geochemical modeling of species present in the water column.

Bare CeO_2-NPs	$[Si(OH)_4]_{TOT}$ = 0.30 mM $[Mg^{2+}]_{TOT}$ = 0.30 mM $[Na^{+}]_{TOT}$ = 0.60 mM $[NO_3^{-}]_{TOT}$ = 0.20 mM $[cit^{3-}]_{TOT}$ = 0.00 $[CO_3^{2-}]_{TOT}$ = 0.20 mM E_H = 0.24 V	$[Ce^{4+}]_{TOT}$ = 36.00 nM $[Ca^{2+}]_{TOT}$ = 0.90 mM $[K^{+}]_{TOT}$ = 0.20 mM $[Cl^{-}]_{TOT}$ = 0.20 mM $[SO_4^{2-}]_{TOT}$ = 0.10 mM $[PO_4^{3-}]_{TOT}$ = 3.80 μM
Coated CeO_2-NPs	$[Si(OH)_4]_{TOT}$ = 0.30 mM $[Mg^{2+}]_{TOT}$ = 0.30 mM $[Na^{+}]_{TOT}$ = 0.60 mM $[NO_3^{-}]_{TOT}$ = 0.20 mM $[cit^{3-}]_{TOT}$ = 0.16 mM $[CO_3^{2-}]_{TOT}$ = 0.20 mM E_H = 0.24 V	$[Ce^{4+}]_{TOT}$ = 0.35 μM $[Ca^{2+}]_{TOT}$ = 0.90 mM $[K^{+}]_{TOT}$ = 0.20 mM $[Cl^{-}]_{TOT}$ = 0.20 mM $[SO_4^{2-}]_{TOT}$ = 0.10 mM $[PO_4^{3-}]_{TOT}$ = 3.80 μM