

## NanoFASE Deliverable D7.1

### Research report on speciation and transformation of NM in soil

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### Research Report Summary

Speciation, for the purpose of this deliverable, is determined as the form in which nanomaterials (NMs) occur in the environment. NM speciation thus has implications for both transport and bioavailability, but also reactivity, e.g. in the context of terrestrial applications such as nano-zerovalent iron (NZVI). This deliverable groups method developments to monitor and quantify speciation in conditions representative of a soil environment and it outlines model approaches for how these speciation changes will be modelled in the overall NanoFASE framework.

Two techniques were tested for quantifying homo- and hetero-aggregation of NMs: nanoparticle tracking analysis (NTA) and field flow fractionation coupled to single particle inductively coupled plasma – mass spectroscopy (FFF-spICP-MS). NTA was useful to monitor hetero-aggregation, but only in specific experimental conditions where the NM in question can be optically discerned from the natural particle with which it hetero-aggregates. Preliminary results showed that FFF-spICP-MS can be used to distinguish between different types of particles, even when they have the same size. However, retention of previous sample in the FFF channel limits the workable concentration range at the lower end (i.e. lower than a few hundreds of  $\text{ng L}^{-1}$ ), while the technique cannot accurately handle too high concentration either (i.e. higher than several  $\mu\text{g L}^{-1}$ ).

Several techniques were tested to monitor redox speciation of NZVI, of which laser Raman scattering proved promising, provided that sample preparation would be enhanced. The technique is, however, only suitable when relatively high concentrations of NMs can be expected.



Model approaches are presented of how speciation changes such as homo- and hetero-aggregation can be integrated within a transport modelling approach. These approaches will be partly based on mechanistic approaches such as DLVO theory for aggregation processes or speciation calculation to take into account the depletion of dissolved ions in soils, which enhances dissolution of NMs.

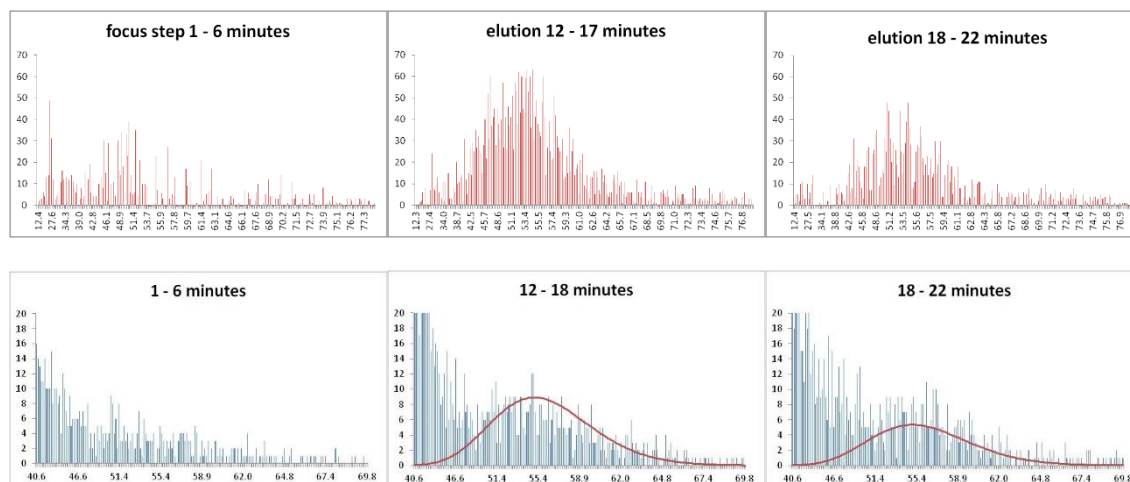


Figure. FFF-spICP-MS analysis of a Ag/Au composite particles. Ag is shown in the upper graphs and Au in the lower ones at different times during the FFF elution, i.e. the focus step (1 – 6 minutes), when the main nanoparticle peak emerged (12 – 18 minutes) and in the tail of the distribution. The tail clearly shows the memory effects of NPs detaching from the FFF membrane, that limit the dynamic range of FFF-spICP-MS. The X-axes show equivalent spherical diameter in (nm), Y-axes show the particle number concentration (mL<sup>-1</sup>).

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