Towards quantitative analysis of magnetic nanoparticle mixtures using COMPASS

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Introduction: Magnetic nanoparticles (MNP) offer great potential for biomedical applications. In particular, the possibility of functionalizing MNPs, i.e. to bind small biomolecules to their surface, makes them a versatile tool [1]. Calculating concentrations from a mixture of different MNP types is an important task since this concept can be translated to the differentiation of MNP with different mobility properties [2]. Among others, this opens possibilities to quantify the binding state of functionalized MNP with a specific biomolecule. Critical Offset Magnetic Particle Spectroscopy (COMPASS) is a suitable method for this task [3]. Here, we analyzed binary mixtures of different sized MNPs via COMPASS measurements using a system matrix approach.

Methods: COMPASS is an extension of conventional magnetic particle spectroscopy (MPS measuring the particles nonlinear magnetization response to an oscillating magnetic field while sweeping through an additional offset field. This provides additional information about MNP magnetization compared to MPS. To reconstruct the concentrations of a particle mixture the following equation must be solved:

$$Ax = b \Leftrightarrow A^{-1}\, b = x, \qquad \text{Eq. 1}$$

where A is the system matrix consisting of the COMPASS signal of 5 particle systems of different sizes (Feraspin™ S (20-30 nm), M (30-40 nm), L (40-50 nm), XL (50-60 nm), XXL (60-70 nm)), x is the concentration and b is the measured signal of the mixed sample. For this experiment, a concentration series of Feraspin™ L and a mixture series of Feraspin™ XL and Feraspin™ S were investigated. For comparison, Singular Value Decomposition (SVD) [4], Kaczmarz algorithm [5] and Non-Negative Least Squares (NNLS) method [6] have been tested.

Results and Discussion: By natively including the condition of nonnegativity of all concentration values, NNLS leads to the best results without requiring any pre knowledge about the particle sample. Figure 1a) shows the reconstruction of the concentration series of Feraspin™ L and Figure 1b) shows the reconstruction of the mixture series of Feraspin™ S and XL. The results show a high level of agreement when compared with the actual concentrations set in the samples.

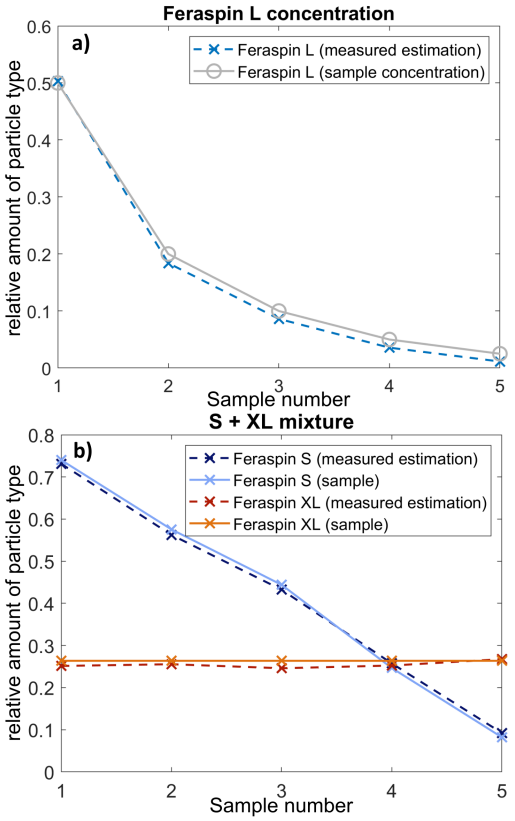

Fig. 1: a) concentration series of Feraspin™ L, reconstructed from a system matrix of five Feraspin™ systems of different size. b) mixture series of Feraspin™ XL and S

Conclusion: It was shown that COMPASS measurements and NNLS based reconstruction enable a good estimation of the concentration of binary MNP mixtures from a system matrix of five different MNP types.

References: [1] Wu, ACS Appl. Nano. Mater. (2020). [2] Viereck, J. Magn. Mater. (2019). [3] Vogel, Nat. Commun. (2022). [4] Hansen, BIT Numer. Math. (1987). [5] Hanke-Bourgeois, Linear Algebra Appl. (1990). [6] Bro, J. Chemom. (1997).