Using Speciation Diagrams to Improve the Design of Magnetic Nanosorbents for Environmental Applications

A. F. C. Campos(1), L. E. C. Benedito(2), F. A. Tourinho(2) and J. Depeyrot(3)

(1) Faculdade UnB – Planaltina, Universidade de Brasília, 73300-000, Brasília (DF), Brazil. e-mail: relex@unb.br
(2) Instituto de Química, Universidade de Brasília – 70919-970 – Brasília (DF) Brazil.
(3) Instituto de Física, Universidade de Brasília – 70919-970 – Brasília (DF) Brazil.

* Corresponding author.

Abstract – This work addresses environmental applications of magnetic nanoparticles. We highlight the chemical design of filtration aids based on specific ligands used in magnetic separation of pollutants from water. Coupling the speciation diagrams of nanoferrites particles surface with that of the ligands, it was possible to provide a theoretical prediction of the optimal pH for particle surface – ligand complexation leading to advances in nanosorbents developing.

Among the numerous promising applications of nanotechnology, there are many that involve the environment. In particular, nanotechnologies play a large role in current efforts to develop better methods for remediation of materials contaminated with hazardous substances. In this context, the procedure of magnetic filtration has been an important tool concerning the process of removal of chemical pollutants from water. However, since most of these contaminants are not magnetic, it is necessary to develop filtration aids to adsorb the pollution agents in order to allow their magnetic separation. These filtration aids can be prepared by coating magnetic nanoparticles with specific ligands which present chemical affinity with the contaminants. Regarding the petrochemicals removal from water, iron oxides nanocomposites based on polydimethylsiloxane (PDMS) have been widely used to coat ferrite magnetic nanoparticles to enhance their adsorption of hydrocarbons. In this process, carboxylic acid-functionalized PDMS are added to the aqueous ferrite nanoparticles dispersion to adsorb the polymer onto the particles surface. Then, as the surface behaves as a diprotic weak acid [1], the ligand binding is strongly dependent on both pH and particle surface charge density. In this way, the aim of this work is to explore, from a theoretical point of view, the oxide particle ligand complexation in order to improve the synthesis of PDMS-complexes used to remove petrochemicals from water. The surface charge density is obtained for magnetic fluids samples based on cobalt ferrite nanoparticles dispersed in water. Then, the speciation diagram of the surface charged sites is coupled with that of the ligands to analyze the mechanism of particle surface – ligand complexation. The obtained results show that the carboxylate groups can bind the nanoparticle surface only in acid pH medium where the surface sites are positively charged. On the other hand, in basic medium the ligands are unable to complex the particle surface. Finally, our approach allows a theoretical prediction of the optimal pH for ligand surface complexation in excellent agreement with reported values [2].

![Figure 1: Coupled speciation diagrams of nanoparticles surface sites (MOH₂⁺, MOH and MO⁻) and PDMS.](image)

References