DESCRIPTION FOR THE GENERAL PUBLIC

Hydroboration reaction is an addition process of the boron-hydrogen bond to the multiple carbon-carbon or carbon-heteroatom bonds. The process, due to its 100% atom economy, high reactivity and low toxicity of organoboron reagents, is the most frequently used in the synthesis of compounds with boryl functions. The boroorganic products can be further used in the synthesis of *fine chemicals*, materials with tailored properties, preceramic materials, active pharmaceutical ingredients (API) or natural products. The stereoselective formation of desired products predominantly requires the use of a catalyst, which accelerates reaction rate, leads to the formation of specific isomers and allows carrying out reactions under milder conditions. Transition metal molecular complexes are still the most used catalyst in hydroboration reactions that occur in homogeneous phase. The catalyst reuse and recycling, easy separation methods of products from the catalyst as well as the sustainability of the whole process are the most challenging tasks in modern organoboron chemistry.

The goal of the project is to deal with these problems by the application of various methods of immobilization of transition metal molecular catalysts or catalysts based on main group elements and nanomaterials and the use of supercritical CO_2 ($scCO_2$) as a reaction solvent. Due to its unique physicochemical properties, $scCO_2$ can be used as a reaction medium and for the development of new catalytic systems for repetitive batch or continuous flow hydroboration. A combination of $scCO_2$ with the molecular catalyst or nanocatalysts immobilization, with the separation strategy responsible for the effective hydroboration processes, constitute an important goal of this project. The project will be focused on understanding the process in all complementary levels: reaction level (interactions between catalyst, solvent and reagents), separation level (development of effective separation strategy of products from catalyst, permitting for its reuse) and process engineering level (the whole process scheme with the monitoring of its progress).

The hydroboration of compounds with the unsaturated C-C or C-heteroatom bonds in $scCO_2$ with the application of molecular catalyst or nanoparticles immobilized in ionic liquid deposited on a solid support (SILP) or using other immobilization methods (the application of ionic liquids, poly(ethylene glycols), hetero polyacid etc.) will constitute the main aspect of the project. The understanding of the whole reaction engineering will allow developing of the repetitive batch and continuous flow hydroboration processes, based on the information gained in all process levels. Taking care of process sustainability, efficiency and economy are one of the most important tasks of innovative processes.

The knowledge gained from the project will build a hub for new organoboron technologies of the 21st century, according to the fundamental research carried out in the project leading to detail process understanding. The project goes beyond the currently realized studies on methods used for hydroboration, catalyst immobilization and the strategies for its recycling, and application of $scCO_2$ as a solvent for sustainable batch and continuous flow synthesis. The project will lead to the development of the first continuous flow processes in the hydroboration of unsaturated carbon-carbon and carbon-heteroatom bonds. The overarching effect of the project will be the design of sustainable processes that will allow the catalyst to be recycled, its good immobilization, the elimination of toxic organic solvents, the simplification of the product separation procedure and the selective synthesis of borylated products (also chiral compounds) with high yields. This approach has the potential to increase the role of homogeneous catalysis in processes with commercial application.