The aim of this work is to design modern, alternative materials with catalytic properties based on carbon nanostructures (CNSs) for model fine chemical production.

The study will involve designing of new materials, characterization and demonstration of their catalytic potential in model chemical processes, like: Baeyer-Villiger oxidation, Diels-Alder cycloaddition and Friedel-Crafts alkylation of aromatics compounds. Due to the importance of the products obtained according to the proposed processes, e.g. monomers, pharmaceuticals and surfactants, efficient methods for their preparation are highly desirable. The obtained results will be used for computer-aided modelling of the Baeyer-Villiger oxidation processes.

The most important features of an effective catalyst is a high activity, selectivity and stability. The main advantage of heterogeneous catalysts i.e. those which form a separate phase in the reaction system, usually solid is simple separation and recycle. Heterogeneous catalysis, although known for over a century, is constantly improved and plays a key role in solving the present problems in chemical technology. Thanks to the development of materials engineering modern, solid catalyst supports having a highly developed surface are available.

In the project authors will design new heterogeneous catalysts and optimize their mechanical, physicochemical and catalytic properties. Appropriate selection of the catalyst components - the active phase and the carrier - may affects its activity, selectivity and stability. It is also important to provide good access of the reactants to the active phase by the expanding of the surface area. Another important issue is the mechanism of immobilization which is the method of depositing of the active phase on a support.

As the catalyst supports carbon nanostructures will be used. CNSs revolutionized the field of nanotechnology, finding use in electronics, optics, mechatronics and as structural components. Specific properties of CNSs, such as high surface area, chemical inertia, the relatively high resistance to oxidation, the ability to make various modifications on the surface make them promising carriers for heterogeneous catalysts.

NCSs will be modified by depositing on their surface of active groups with catalytic capability in the form of acidic ionic liquids (ILs). The deposition will take place by adsorption of the active phase or by chemical bond to the carrier. The latter approach is more efficient and prevents leaching of the active phase in the process, during separation and recycle of the catalyst. Adsorption of ILs on the surface of CNSs is one method of improving the dispersibility of the catalyst in the reaction system. The combination of high catalytic potential of ionic liquids with excellent carrier properties leads to a hybrid materials with innovative properties.

For the preparation of heterogeneous catalysts we will use carbon nanostructures (CNSs), i.e. pristine and surface-modified single- and multi-wall carbon nanotubes, as well as other CNSs – carbon nanofibers, carbon nanoonions, graphenoid structures. Moreover, an integral feature of some of the proposed nanomaterials will be the presence in their cores irremovable via chemical modifications superpara- and ferromagnetic iron nanoparticles. This characteristics allows for an easy removal of catalysts from the post-reaction mixtures by means of magnetic field which is a significant advantage in the light of economy of processing.

It is worth noting that the use of hybrid materials: carbon nanomaterial-ionic liquid (CNSs-ILs) as catalysts in chemical processes previously has been described in a few works. It has been shown that the use of CNSs as an ionic liquid phase carriers brought many advantages over conventional oxide carriers. A high catalytic activity is the result of the use of mesoporous support, which improves the mass transfer.

In this project we have chosen three model processes for catalytic tests: Baeyer-Villiger oxidation, Diels-Alder cycloaddition and alkylation of aromatic compounds to study the catalytic performance of our new catalysts. The studies under the favourable conditions e.g. temperature, concentration of reagents, the amount of catalyst, and solvent selection will be realized. The reaction calorimeter equipped with FTIR control probe allows us tracking of the process and the assignation of kinetics and heat of the process. All catalysts will be characterized by high hydrolytic stability that solve existing problems in the test reactions with the application of Lewis catalysts that undergo rapid hydrolysis even in the presence of trace amounts of water.

Modern methods of processes design increasingly rely on modeling and optimization using mathematical modeling and computer simulation. Application of the ChemCAD program as a modern tool of chemical engineering culminate the project. It allows for detailed analysis of the process, determine the equations of mass and energy balance of the process.

In conclusion, the search for new highly effective, yet non-toxic, environmentally friendly catalysts are currently the object of many studies. The proposed project involves the use of new, yet poorly known heterogeneous catalysts based on hybrid materials constructed from a combination of carbon nanomaterials and ionic liquids for model chemical processes.