

Currently, the main interest of industrial biotechnology is production of valuable compounds with high efficiency, however at low cost and in a short processing time. Therefore, the practical use of immobilized enzymes finds profound economic justification. Besides binding to insoluble carriers and crosslinking, the inclusion of enzymes (e.g. in hydrogel structures) is one of the basic types of immobilization. This method is cheap, fast and enables to obtain active preparations with enhanced stability, without significant influence on the changes in the native structure of entrapped enzymes. Nevertheless, numerous studies on immobilization of enzymes in hydrogel matrices (described in the literature) are limited only to determination of the property profile of given biocatalyst as a function of estimated parameter (e.g. pH, temperature). Such information is required to design bioreactors facilitating economical use of enzyme, which is often the most expensive component of the process. In general, there is a lack of information about probable causes of the changes in the properties of the biocatalyst after inclusion in hydrogel lattice, which would have been explained on the molecular level. Among others, in this case, it has not been examined the effect of chemical composition, physical properties and the degree of crosslinking of polymeric matrix on the immobilization efficiency obtained for given enzyme. There are only a few reports related to molecular modeling of spatial structures for selected hydrogel materials

The main goal of the project is the recognition, explanation and description of the quantitative interactions occurring in the hydrogel matrix of different chemical composition and and the correlation of these interactions with the change in the properties of given biocatalyst after immobilization, which are necessary in designing of bioreactor processes.

The project has an interdisciplinary nature and mainly includes research issues in the field of bioprocess engineering, material science and molecular modeling. It presents the series of experimental studies related to preparation and characteristics of hydrogel matrices, selection of immobilization conditions and determination of the properties of selected enzymes after entrapment. Besides strictly experimental approach we apply a comprehensive multiscale modeling, aimed at identifying and quantitative description of interactions arising in the given hydrogel matrix (depending on its chemical composition) and linking of determined parameters with the results obtained experimentally.

It is predicted that ultimate result, that obtained results enable the selection such hydrogel carrier for given enzyme, that will ensure optimal use of its catalytic properties. Furthermore, using numerical methods to preliminary design of the most effective enzyme - hydrogel system, the expensive and time-consuming experiments could be limited to verification in the narrower range of tested parameters (close to the optimum values).