

Many aspects of life in the 20th and 21st century were dominated by issues related to catalysis. Moreover, modern industry strives to produce chemical compounds in accordance with the principles of green chemistry. In those regards, the synthesis of chiral compounds like cyanohydrins and β -nitro alcohols, which are used to synthesise α -hydroxyaldehydes, ketones and β -aminoalcohols and many more is of particular interest. This is due to the fact that these compounds are used as precursors for obtaining very important substances in sectors of modern industry related to pharmacy, cosmetics and food chemistry. These compounds can be obtained from relatively inexpensive and widely available chemicals like toluene and benzyl alcohol via cascade processes that combine photocatalysis and biocatalysis. Integrating enzymatic catalysis and photocatalysis in these processes allows their advantages to be used synergistically. However, one of the most crucial challenges in implementing these processes is ensuring the compatibility of enzymes with the conditions of the photocatalytic process, such as the presence of reactive oxygen species, intense UV radiation or changes in pH. Therefore, within the framework of the current project we intend to undertake original research work, both experimental and theoretical (modelling), primarily in order to acquire new knowledge about the foundations of observable phenomena in the newly developed reactor system design. In particular, we aim to address the identified challenges by developing an effective cascade process for synthesising chiral cyanohydrins and β -nitro alcohols using immobilised photocatalysts such as anthraquinones or titanium dioxide (TiO₂), and immobilised enzymes from the hydroxynitrile lyases group.

Monoliths and silica coatings will be obtained using the sol-gel method and then modified in a post-synthesis procedure. Enzymes will be immobilised by a covalent or metal binding. An extensive characterization of all the prepared materials/catalysts will be carried out to allow for the determination of structure-activity/performance relationship. The activity of the photocatalysts and the immobilized enzymes will be checked in the test reactions using flow reactors. The hydrodynamic aspects of the enzymatic and photocatalytic flow reactors will be investigated as well based on experimental measurement results combined with numerical analysis. For simulations ANSYS Fluent as the CFD solver will be used running on a specially dedicated computing server.

From a chemical and process engineering perspective, research activities in the field of multicyclic/cascade reaction systems predominantly focus on batch (periodic) reactions in homogeneous or two-phase systems. Reports on the application of heterogeneous (immobilised) catalysts are scarce, and there are none at all on dedicated to continuous flow modes of operation. Using the application of immobilised catalysts enables the reaction to be stopped at any time, allowing the catalyst to be reused. In the case of biological catalysts, this also typically results in improved enzyme stability during the reaction. Most heterogeneous catalysts are employed in batch processes involving mechanically stirred tank reactors. However, one of the disadvantages of this method is the gradual degradation of the catalyst grain. Furthermore, the need to ensure intensive mass transfer in the suspension limits the amount of heterogeneous catalyst that can be used, which directly affects the efficiency of the process. In addition, upscaling in batch applications causes problems relating to heat and mass transfer, as well as mixing. Scale transfer issues in tank reactors are particularly significant for photocatalytic processes, given the limited penetration depth of incident light when the amount of catalyst and the reactor volume are increased. This leads to a sharp decrease in irradiation efficiency and reduced catalyst utilisation, resulting in an unsatisfactory yield and selectivity of the target product. The limitations of batch systems are discussed here in order shown to highlight the need for development of a specialised flow system with a high surface-to-volume ratio and an effective distribution strategy for the heterogeneous photocatalyst, paving the way for practical applications. A continuous microflow reactor can achieve uniform and effective light irradiation using narrow-diameter tubing or microchannels. Other advantages of continuous microflow reactors include improved mass and heat transfer, enhanced safety, precise control of reaction parameters, excellent reproducibility and ease of scaling up. Equally important for achieving optimal process parameters is the development of appropriately designed catalysts and specialised reaction systems (reactor). Therefore, we are convinced that both above mentioned modifications could greatly improve the efficacy of reaction systems, making them more cost-effective and biomimetic (combining the effects of physical proximity, co-localisation and space confinement, which are typical of cells).

The research work undertaken in this project will help to significantly develop the knowledge on innovative reactor systems, allowing to determine kinetic and process parameters enabling the integration of the biocatalytic module with the photocatalytic one. As a consequence, these modifications may lead to the identification of possibilities for improvement the efficacy of catalytic systems in the future, making them more cost-effective and biomimetic.