The studies foreseen in the project concern very challenging problem of organic technology regarding a searching for new, efficient heterogeneous catalyst of one step synthesis of propylene oxide (PO). Always growing demand for this compound applied for the production of propylene glycols, polyurethane, polyether polyols, and other compounds require novel, more efficient and environmentally friendly technologies. An annual worldwide production of PO is approximately 7.5 million tons.

Propene oxide is currently produced using two different types of processes: the chlorhydrin process and the hydroperoxide process. Because of the environmental impacts the most recently built plants are using hydroperoxide technologies. However, a disadvantage of the above processes resulting in the production of a co-product (either styrene or tert-butyl alcohol, depending on the kind of the hydroperoxide process) formed in a volume that is 3 times larger than that of propene oxide, the economy of the process is primarily dominated by the market of the co-product. Therefore, research effort is focused on the development of alternative, direct epoxidation processes for the production of propene oxide. The aim is to develop a process for the direct gas-phase oxidation, similar to the direct epoxidation of ethene. However, the catalysts, that have been developed for the direct epoxidation of propene using oxygen or air, are not efficient enough to be used commercially.

Recently, we have found for the first time that vanadium catalysts supported on silica support show noticeable activity in propene epoxidation when N_2O was used as an oxidant. Even more important was revealed that instead of propene, propane can be also oxidized in one step to propene oxide. The use of propane, instead of propene, as a starting material for propylene oxide production, is of a special interest due to the elimination of the costly step of propane to propene transformation. This findings encouraged us to more detailed searching for the modification of the vanadium based catalytic system for one step propylene oxide manufacturing.

The modified vanadium catalysts supported on mesoporous silica matrices will be applied in the proposed project for propane and propene epoxidation using N_2O as an oxidant. As a modifier we are planning to use alkaline metal ions (Na, K, Rb and Cs) in order to diminish catalysts acidity, as the acidic sites are responsible for propylene oxide isomerization, and subsequently in lower yield of PO. Apart from alkaline ions, we will also introduce other metals (Fe, Mo and Sb) which were reported in literature as an active component of vanadium catalysts applied for oxidation reaction. The increase of propylene oxide productivity on the modified vanadium-based catalytic system is expected.

We have found in our preliminary studies the possibility of direct processing of propane to propylene oxide, however, the propane conversion decreased fast due to reduction of vanadium species and this catalytic system cannot be considered for industrial application. Therefore, apparat from catalysts modification, the use of a mixture of oxidants (N_2O and O_2) instead of pure N_2O will be applied. Since the presence of oxygen enable faster reoxidation of vanadium catalysts, the limitation of propane conversion decrease is expected. Another approach to limit the decrease of propane conversion will be application of vanadium catalysts modified with sulphate groups, which facilitate the reoxidation of V^{4+} to V^{5+}.

The obtained catalysts will be broadly characterized with various physico-chemical techniques. All catalysts will be examined in the reaction of one step oxidation of propane and propene performed under atmospheric pressure. The reaction will be carried out at different temperatures (in the range of 623K – 703K), using pure N_2O, or the mixture of N_2O/O_2 as the oxidants.

We expect to obtain active and stable catalyst for one step epoxidation of propane and propene which could be considered an alternative to the currently used commercial methods of propylene oxide manufacturing.