The project is on investigation of the phenomenon of modulation of turbulence by droplets present in the semi-dilute and concentrated emulsions. It is well known that the presence of droplets of the dispersed phase affects micro-flows within and outside the droplets, and such micro-flows cause changes in the droplet shape and possibly break up the droplets. Viscosity of dense emulsions is high and variation of the drop size and shape significantly alters it. This in turn affects character and velocity distribution of the main flow. However, this is not the only effect of micro-flows, because the movements of small drops affect mixing of species in the continuous phase as well as mass transfer between the dispersed and continuous phase. All these phenomena are responsible for contacting reactants, so they affect the course of the complex chemical reactions and the resulting product distribution. Research project objectives are defined as theoretical interpretation of interactions of the micro- and nano-scale phenomena with the above mentioned effects observed at macro-scale, development of adequate mathematical models and validation of theories and models by performing experimental investigations.

Proposed investigations are based on linking advanced theoretical approach and methods of modeling (theoretical models, CFD) with experimental investigations. Investigations of chemical reactions in the fluid present between droplets of emulsions should enable testing of different models of microflows around and within droplets, including these proposed in present project, as well as their effect on contacting reactants. Because the structure of emulsion affects its viscosity, important information especially in the case of dense emulsions, one can obtain based on rheological investigations. For dilute emulsions the LDA measurements can be carried out. Evolution of the drop size will be investigated using laser particle analyser for micro-droplets and the scanning mobility particle sizer (Multisizer) as well as the scanning electron microscopy (SEM) for measuring the size distribution and shape of nano-droplets. The method of modeling should enable to follow changes in the drop size distribution as the result of action of turbulent stresses, express the viscosity of emulsion as a function of the drop size distribution and concentration of the dispersed phase, and finally show how rheology affects the main flow and how the turbulent stresses are created in emulsion. Simulations will be performed using CFD: volume of fluid (VOF) model will be used to simulate drop deformation, breakage, internal and external microflows, interaction of droplets and to identify mass transfer coefficients, internal and external, whereas RANS models will be used to simulate large scale flows, mixing and chemical reactions. The CFD models will be supplemented with the user defined functions (UDF) for drop size distribution and media properties dependent rheology, breakage kernels, time constants for mixing, and closure schemes for turbulent flow and fast chemical reactions.

The complex chemical reactions will be used as the test reactions in the project, to investigate energetic efficiency of mixing in multiphase systems. Using test reactions one can characterize the level of mixedness (intensity of segregation, time constants for mixing, the rate of interfacial mass transfer) and use this information to validate theoretical models and improve performance of processes carried out in chemical reactors and mixers.

Practical aspects of proposed project are related to carrying out the complex chemical reactions at high selectivity. Based on results of this project a better design and performance of chemical reactors should enable to run chemical reactions with the highest possible selectivity with positive effect on environment protection. Notice that purification of chemical products is costly, hence results of proposed project can have economical aspects as well.