An integral feature of the surrounding nature and technology is enormous complexity and diversity of the processes that take place. We can say that there is nothing constant in the world. Even relatively simple chemical and biological systems may exhibit very complex dynamic behavior. Due to diversity of the behaviors and a large number of the parameters that characterize each system, a comprehensive analysis of the phenomena that may be encountered is usually possible only by using appropriate tools of mathematical modeling and computer simulation. However, when using these tools we must remember that the mathematical model is only an artificial formation created by the researcher, and therefore it may have some characteristics that the real system does not possess. As a result, it is necessary to verify the results of the simulations with the reality.

Relatively new technological concept in chemical engineering are so-called multifuctional or hybrid catalyst pellets. They allow to carry out several physical and chemical processes in a single apparatus. The integration of chemical reaction and product adsorption or of several chemical reactions in a single chemical reactor usually is done on a macroscale. This means that the processes take place in a mixture of adsorbent and catalyst pellets or in a mixture of different catalysts. The main characteristic of hybrid pellets is the combination of these two materials in a single particle. Such synergy may ultimately improve the efficiency of a given process. The complexity of mechanisms taking place in catalytic and adsorptive reactors combined with dynamic nature of the pellets suggest that the dynamics of such objects may be very complex. Analysis of the dynamics of hybrid pellets is essential, primarily due to their potential application in many chemical processes.

The aim of the project is broadening of theoretical knowledge concerning the dynamics of multifunctional catalyst pellets and selected types of catalytic and adsorptive reactors. This knowledge is essential for further theoretical and empirical research on the design of multifunctional pellets and of adsorptive and catalytic reactors as well as for the proper selection of operating conditions and dynamic control of the existing apparatuses. The comprehensive analysis of the dynamics of pellets and multifunctional reactors requires the construction of complex mathematical models that account for the most important physicochemical phenomena and the application of numerical methods necessary to develop simulation codes. Simulations of the dynamics of the formulated mathematical models will be performed based on the selected approximation methods allowing to reduce the model order, which significantly advanced over the last decade. The approximation methods enable to reduce significantly the computational time significantly while maintaining the accuracy. Theoretical evaluation of the benefits of using hybrid pellets will be supplemented with verification of the results of numerical simulations with experimental data taken from the literature.