Name of the course	**Chemical reactor analysis and modeling**
Number of instruction hours	20
Outline of course/module content	Kinetic analysis and selection of the experimental reactor. Basic types of experimental reactors – integral, differential, gradientless and microreactors. Methods of kinetic analysis and treatment of the experimental data. Choice of model and parameters estimation. Application of ID algorithm (exchanged differential method) for parameter estimation of complex kinetic models. Chemical reactor as the process space. Development of the mathematical models based on the physical features and assumptions about dependences of state variables and parameters on the reactor�s space and time. Analysis of the complex impact of the reaction kinetics and mass transfer models on the complexity of the reactor model. Analysis of the mass transfer with simultaneous chemical reaction and heat transfer in the real systems. Modeling of the complex reactive systems. Analysis and modeling of multiphase reactors. Reactor optimization with respect to the number of participating reactions and temperature regime. Residence time distribution, stability and selectivity, stationary and dynamic operation of the reactors. Numerical methods of solving the models with partial differential equations. Examples: the pseudohomogeneous two-dimensional model of tubular fixed bed reactor, model of the photocatalytic reactor, model of the multiphase gas - liquid reactor (bubble column). Case studies of the advanced (structured) design of reactors: microreactors and monolithic reactors. Microreactors: Introduction to Micro-Reactor Technology (MRT), „state of the art“, definition of microscale reactor, fundamental advantages of microscale chemical processes, microscale reactors areas of application, modern microfabrication techniques. Fluid flow in a microchannel. Reaction-diffusion dynamics in microreactor. Numerical experiments and analysis. Examples: steroid extraction in a microchannel system - mathematical modelling and experiments, lipase-catalyzed synthesis of isoamyl acetate in a microreactor, microreactor and ionic liquids. Monolith reactors: Monolith structures, materials and properties. Comparison with conventional catalytic reactors. Clasification and application of monolithic reactors. Emerging applications (hydrogen generation for the fuel cell, steam reforming of hydrocarbons, fast catalyst screening and kinetic studies). Hydrodynamics, heat and mass transfer in monoliths, kinetics and pressure drop. Modeling of monolith reactors. Examples: comparison of 1D and 2D heterogeneous models of the monolith reactor for catalytic reduction of nitrogen oxides (NOX).
Description of instruction methods	oral, seminar, consultations
Description of course/module requirements	completion of seminar work