

<b>Elective Lecture</b>					
<b>Module number</b>	<b>Credits</b>	<b>Workload</b>	<b>Term</b>	<b>Frequency</b>	<b>Duration</b>
	5 CP	150 h	2. Sem.	only SoS	1 Semester
<b>Courses</b> Modern Microkinetics			<b>Contact hours</b> a) 2 SWS b) 1 SWS	<b>Self-Study</b> 105 h	<b>Group size</b> All students choosing Industrial Chemistry
<b>Prerequisites</b> Solid knowledge of basics in <i>Chemical Reaction Engineering</i> , Industrial Chemistry and Physical Chemistry					
<b>Learning outcomes</b> <ul style="list-style-type: none"> <li>• By means of examples students acquire advanced knowledge on basics and application of modern simulation tools used in chemical engineering. The kinetics of a reaction is described based on elementary steps. After the course students are able to solve basic problems of chemical reaction engineering using MATLAB.</li> <li>• Soft skills: interactive presentation in front of an audience, notetaking during lectures, unsolicited post-preparation of module contents, unsolicited consultation of the relevant literature</li> </ul>					
<b>Content</b> <ol style="list-style-type: none"> <li>1. Modeling a chemical reaction using elementary steps: introduction of microkinetic modeling, description of adsorption, desorption and reaction on a molecular basis, statistical thermodynamics, estimation of kinetic parameters, modeling of temperature-programmed experiments, simulation of SSITKA experiments</li> <li>2. Microkinetic models: determination of kinetic parameters, Levenberg-Marquardt algorithm, examples</li> <li>3. Reactor models: adiabatic packed-bed reactors, heterogeneous and pseudo-homogeneous models, consideration of non-steady reactor states, model selection, programs of estimation of kinetic constants</li> <li>4. numerical tools for solution of non-linear algebraic equations and non-linear differential equations: boundary and initial value problems, one- and multiple-step procedure</li> <li>5. overview of commercial software and routines in numerical/statistical libraries, introduction to MATLAB</li> </ol>					
<b>Teaching methods</b> a) Lecture; b) Exercises using MATLAB					
<b>Mode of assessment</b> 30 min end-of-term oral exam					
<b>Requirement for the award of credit points</b> Passing the oral exam					
<b>Module applicability</b> Master of Chemistry, focal point Industrial Chemistry					
<b>Weight of the mark for the final score</b> Weighted according to CPs					
<b>Module coordinator and lecturer(s)</b> M. Muhler, B. Mei					
<b>Further information</b> All documents are provided via <i>moodle</i>					