UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	IZBRANA POGLAVJA IZ KEMIJSKEGA REAKCIJSKEGA INŽENIRSTVA
Course Title:	SELECTED TOPICS IN CHEMICAL REACTION ENGINEERING

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
DR Kemijske znanosti, 3. stopnja	**/**	**1.**	**1. in 2.**
Doctoral programme in Chemical Sciences, 3rd Cycle	**/**	**1st**	**1st and 2nd**

Vrsta predmeta / Course Type: izbirni/Elective

Univerzitetna koda predmeta / University Course Code: KZ314

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
15	**45**	**/**	**/**	**30**	**60**	**5**

Nosilec predmeta / Lecturer: prof. dr. Matjaž Krajnc /Dr. Matjaž Krajnc, Professor

Jeziki / Languages:

Predavanja / Lectures:	**slovenski / Slovenian**
Vaje / Tutorial:	**slovenski / Slovenian**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	Prerequisites:
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	Content (Syllabus outline):
Kataliza. Trdni katalizatorji. Teorija reakcijske hitrosti. Reaktivnost površine. Modeli kemisorpcije. Mehanizmi in kinetika heterogeno kataliziranih reakcij. Heterogeno katalizirane reakcije oksidacije in redukcije (hidrogeniranje). Asimetrična kataliza. Heterogene katalitske reakcije v superkritičnih fluidih in ionskih tekočinah. Večfunkcionalni katalizatorji. Deaktivacija katalizatorjev. Kataliza na področju varstva okolja. Aplikacije v petrokemični in farmacevtski industriji. Večfazni reaktorji z eno reakcijo. Vpliv transporta snovi in toplote pri reakcijah na	Catalysis. Solid catalysts. Reaction rate theory. Surface reactivity. Models of chemisorption. Mechanisms and kinetics of heterogeneous catalyzed reaction. Catalytic oxidation and reduction (hydrogenation) reactions. Asymmetric heterogeneous catalysis. Heterogeneously catalyzed reactions in supercritical fluids and ionic liquids. Multifunctional catalysts. Catalyst deactivaion. Environmental catalysis. Application in petrochemical and pharmaceutical industry. Multiphase reactors: single reactions. The role of mass and heat transfer at the surface

zunanji površini in znotraj poroznega katalizatorja. Modeli reaktorjev za študij snovnega transporta v heterogenih sistemih (plin-kapljevina, kapljevina-kapljevina, fluid-trdno). Določitev transportnih koeficientov v večfaznih reaktorjih. Večfazni reaktorji s kompleksno reakcijsko shemo. Simultani transport dveh reaktantov pri neodvisnih in odvisnih paralelnih reakcijah. Snovni transport pri konsekutivnih reakcijah. Snovni transport pri paralelno-konsekutivnih reakcijah. Toplotni efekti v večfaznih reaktorjih. Reaktorji plin-kapljevina: kolona z mehurčki, reaktorji z mešalom. Reaktorji plin-trdno: katalitski in nekatalitski. Reaktorji plin-kapljevina-trdno.	reactions and within the porous catalyst. Model reactors for studying mass transfer with chemical reactions in heterogeneous systems: gas-liquid, liquid-liquid, fluid-solid. Measurement techniques for mass transfer coefficients in multiphase reactors. Multiphase reactors: multiple reactions. Simultaneous mass transfer of two reactants with independent and dependent parallel reactions. Simultaneous mass transfer with consecutive reactions. Mass transfer with mixed parallel and consecutive reactions. Heat effects in multiphase reators. Gas-liquid reactors. Bubble column and agitated reactors. Gas-solid reactors. Gas-liquid-solid reactors.

Temeljna literatura in viri / Readings:

- I. Chorkendorff and J.W. Niemantsverdriet: *Concept of Modern Catalysis and Kinetics*, 2. izdaja, Wiley-VCH, Weinheim, 2007.
- G.F. Froment and K.B. Bischoff: *Chemical Reactor Analysis and Design*. 2. izdaja. John Wiley & Sons, New York, 1990.
- Članki v vodilni kemijsko-inženirski periodiki, npr. *AIChE Journal*, *Chem. Eng. Sci*., *Ind. Eng. Chem. Res*. in drugih.

Cilji in kompetence:	**Objectives and Competences:**
Študent poglobljeno spoznava interakcije med kinetiko reakcij na površini trdnega katalizatorja in transportnimi pojavi v reakcijskih sistemih z več fazami. Pridobljena znanja mu omogočajo: (i) interpretacijo eksperimentalnih rezultatov o poteku ene in ali več reakcij vodenih v večfaznih reaktorjih in (ii) optimalno načrtovati in upravljati večfazne reaktorje, ki jih pogosto najdemo v farmacevtski in sorodni industriji. Ta znanja študenta kvalificirajo tudi za samo izbiro procesa oziroma tipa reaktorja, ki bo zagotavljal želeno selektivnost in dobitek in pri študentu spodbujajo kritično uporabo osvojenih znanj za reševanje inženirskih problemov pri uvajanju sodobne procesne intenzifikacije.	Students gain deeper insight into the interaction between transport phenomena and kinetics of chemical reactions taking place on solid catalysts. These knowledge help them to: (i) quantitatively interpret the experimental kinetic data obtained in a multiphase reactor and (ii) optimally design and operate multiphase reactors such as frequently employed in pharmaceutical and related industry. Students are qualified to select the most appropriate reactor for achieving the highest selectivity and production of the desired products as well as to use their knowledge critically in order to solve more complex engineering problems for process intensification.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Študent zna samostojno preučevati znanstveno literaturo s področja reakcijskega inženirstva. Pridobi poglobljena znanja o izbrani tematiki.	Knowledge and Comprehension Student comprehends scientific literature in the field of reaction engineering. Gains specific and detailed knowledge on selected topics.
Uporaba Pridobljena znanja in uporabljene pristope je sposoben uporabiti pri samostojnem razvojnem in raziskovalnem delu na področju reakcijskega inženirstva.	Application Acquired knowledge and used approaches are necessary for independent research and development in the field of reaction engineering.
Refleksija Študent je sposoben samostojno definirati problem, načrtovati vsebino raziskovalnega dela, predvideti metode dela ter postaviti raziskovalne cilje.	Analysis Student is able to define problems, propose the content of a research project, suggest research methods and state its goals.
Prenosljive spretnosti Študent je sposoben kritično analizirati in povezovati literaturne podatke, sintetizirati različna znanja, zagovarjati rezultate ter sodelovati v diskusiji.	Skill-transference Ability Ability to critically interpret and interconnect literature data, to synthesize knowledge, to defend project results and to discuss them.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Uvodi v vsebinske sklope kot predavanja. Večina kontaktnih ur kot seminar. Zahteva tudi veliko dela doma pri pripravi projekta in seminarja. Razprava pri predstavitvah seminarjev in projektov – oblikovanje skupine oponentov za vsak projekt posebej	Lectures as introductions to various topic modules. Contact hours in forms of a seminar. Independent work in preparing projects and seminars. Active participation in discussion during project/seminar presentations – formation of a group of opponents for every project.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Predloženo poročilo o projektem delu v pisni obliki. Ustni zagovor projektne naloge.	**50** **50**	Written project report. Oral project defence.

Reference nosilca / Lecturer's references:

- RUČIGAJ, Aleš, KRAJNC, Matjaž. Kinetic modeling of a crude DERA lysate-catalyzed process in synthesis of statin intermediates. *The chemical engineering journal*, ISSN 1385-8947. [Print ed.], 2015, vol 259, no. 1,
- RUČIGAJ, Aleš, KRAJNC, Matjaž. Optimization of a crude DERA lyzate-catalyzed process in synthesis of statin intermediates. *Organic process research & development*, ISSN 1083-6160, 2013, vol. 17, no. 5, str. 854-862,
- ŠINKOVEC, Ervin, POHAR, Andrej, KRAJNC, Matjaž. Phase transfer catalyzed esterification : modeling and experimental studies in a microreactor under parallel flow conditions. *Microfluidics and nanofluidics*, ISSN 1613-4982, 2013, vol. 14, no. 3/4, str. 489-498,

- ŠINKOVEC, Ervin, KRAJNC, Matjaž. Phase transfer catalyzed Wittig reaction in the microtube reactor under liquid-liquid slug-flow pattern. *Organic process research & development*, ISSN 1083-6160, 2011, vol. 15, no. 4, str. 817-823,
- LIKOZAR, Blaž, KRAJNC, Matjaž. Cross-linking of polymers : kinetics and transport phenomena. *Industrial & engineering chemistry research*, ISSN 0888-5885. [Print ed.], 2011, vol. 50, no. 3, str. 1558-1570,