

UČNI NAČRT PREDMETA / COURSE SYLLABUS

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| Predmet: | KATALIZA IN HETEROGENI REAKCIJSKI SISTEMI |
| Course Title: | CATALYSIS AND HETEROGENEOUS REACTION SYSTEMS |

| Študijski program in stopnja Study Programme and Level | Študijska smer Study Field | Letnik Academic Year | Semester Semester |
|---|-------------------------------|-------------------------|----------------------|
| MAG Kemijsko inženirstvo, 2. stopnja | / | 1. | 1. |
| USP Chemical Engineering, 2 nd Cycle | / | 1 st | 1 st |

Vrsta predmeta / Course Type:

obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code:

IN211

| Predavanja Lectures | Seminar Seminar | Vaje Tutorial | Klinične vaje Work | Druge oblike študija | Samost. delo Individual Work | ECTS |
|------------------------|--------------------|------------------|-----------------------|-------------------------|---------------------------------|------|
| 60 | 15 | / | / | / | 75 | 5 |

Nosilec predmeta / Lecturer:

prof. dr. Matjaž Krajnc / Dr. Matjaž Krajnc, Full Professor

Jeziki / Languages:

Predavanja / Lectures: slovenski / Slovenian

Vaje / Tutorial: slovenski / Slovenian

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:

Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.

Prerequisites:

The course has to be assigned to the student.

Vsebina:

- Mehanizmi reakcij na površini trdnega katalizatorja. Kinetika reakcij na površini. Teorija prehodnega stanja površinskih reakcij. Reaktivnost površine.
- Karakterizacija trdnih katalizatorjev. Katalizatorji v farmacevtski in petrokemični industriji ter katalizatorji v procesih varstva okolja.
- Transport snovi in toplote na površino trdnega katalizatorja,
- Transport snovi in toplote znotraj poroznega katalizatorja. Efektivnostni faktor in globalna hitrost reakcije.
- Eksperimentalno določanje kinetičnih enačb za katalitske reakcije.
- Analiza in načrtovanje reaktorjev za katalitske

Content (Syllabus outline):

- Reaction mechanisms on the surface of solid catalysts. Reaction kinetics on the surface. Theory of the transition state of surface reactions.
- Characterization of solid catalysts. Catalysts in pharmaceutical and petrochemical industries and catalysts in the processes of environmental protection.
- Heat and mass transfer to the surface of solid catalyst,
- Heat and mass transfer within a porous catalyst. Effectiveness factor and global rate of reaction.
- Experimental determination of kinetic equations for catalytic reactions.
- Analysis and design of reactors for catalytic reactions. Pseudo-homogenous and heterogeneous models. Fixed-bed reactor.

reakcije. Psevdo-homogeni in heterogeni modeli. Reaktor s strnjenim slojem. Kapalni reaktor. Reaktor z goščo. Reaktor s fluidiziranim slojem. Adiabatni reaktor s strnjenim slojem in stabilno obratovanje.

- Heterogene nekatalitske reakcije. Reakcija v sistemu kapljevina-kapljevina in kapljevina-trdno. Reakcija v sistemu plin-kapljevina.

Načrtovanje reaktorjev za nekatalitske heterogene reakcije.

Trickle-bed reactor. Slurry reactor. Fluidized-bed reactor. Fixed-bed adiabatic reactor and stable operation.

- Heterogeneous non-catalytic reactions. Reactions in fluid-fluid, fluid-solid, and gas-fluid systems. Designing reactors for non-catalytic heterogeneous reactions.

Temeljna literatura in viri / Readings:

- G.F. Froment and K. B. Bischoff, Chemical Reactor Analysis and Design, 2. izdaja, Wiley, 1990, 661 strani (70 %)

- I. Chorkendorff and J.W. Niemantsverdriet, Concept of Modern Catalysis, 2. izdaja, Wiley-VCH Verlag, 2007, 457 strani (30 %)

Cilji in kompetence:

Predmet študentu razvija sposobnost analize in sinteze kompleksnih procesov s snovno pretvorbo (reakcijo). Predmet je nadaljevanje predmeta Kemijsko reakcijsko inženirstvo in ponuja znanja, ki so potrebna pri obravnavanju in načrtovanju procesov ter reaktorjev, v katerih potekajo reakcije z več fazami. Specifične kompetence predmeta so:

- poznavanje, razumevanje in uporaba zakonov o ohranitvi mase, energije in gibalne količine, ko se kemijske pretvorbe odvijajo v večfaznem sistemu.
- poznavanje, razumevanje in uporaba matematičnih zapisov hitrosti kemijskih pretvorb v heterogenih sistemih,
- poznavanje in uporaba zvez med transportom toplote in snovi med fazami ter hitrostjo zginevanja snovi na površini katalizatorja,
- poznavanje in uporaba zvez med notranjim transportom in hitrostjo reakcije znotraj poroznega katalizatorja

Objectives and Competences:

Developing competences for carrying out analysis and synthesis of complex reaction processes. The course is a follow-up to the Chemical reaction engineering course and provides the knowledge that is necessary for planning and designing processes in multi-phase reactors. Subject-specific competences include:

- understanding and applying the laws of mass preservation, energy, and momentum when chemical changes occur in multi-phase systems,
- understanding and applying mathematical descriptions of the rate of chemical changes in heterogeneous systems,
- understanding and applying correlations of heat and mass transfer between the phases and the rate of mass disappearance at the catalyst surface,
- understanding and applying correlations between internal transport and the rate of reaction within a porous catalyst.

Predvideni študijski rezultati:

Znanje in razumevanje
Študent spozna osnovne zakonitosti v zapisovanju hitrosti kemijskih in fizikalnih sprememb na infinitesimalni ravni reaktorja vendar na molekularni skali. Razume, da le

Intended Learning Outcomes:

Knowledge and Comprehension
Student becomes aware of fundamental principles of formulating the rate laws on the molecular level within the infinitesimal reactor volume. He understands that the integration over the whole

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| integracija po prostoru reaktorja daje zvezo med obratovalnimi pogoji in dobitkom na makro skali. | reactor space provides the performance equation(s), which relates the operational conditions to the reactor yield. |
| <u>Uporaba</u> Ta znanja mu omogočajo analizo obratovanja obstoječih in načrtovanje novih reaktorjev za vodenje enostavnih reakcij in reakcij v sistemu z več fazami. | <u>Application</u> Possessing sufficient fundamental knowledge student can analyze the operation of simple existing reactors and understand the design of a new one. |
| <u>Refleksija</u> Študent je sposoben povezati znanja iz matematike, fizike, kemije, transportnih pojavov in pridobiti poglobljeno sliko o dogajanju v reaktorju na mikro nivoju. Pri zahtevnem načrtovanju kemijskih reaktorjev in drugih procesnih naprav, je ta sposobnost potrebna tudi za komuniciranje/sodelovanje z drugimi tehniškimi strokovnjaki. | <u>Analysis</u> Student is capable of using the knowledge of chemical kinetics and transport phenomena to formulate the reactor model and thus obtain a deeper insight on the processes on micro as well as macro reactor scale. This ability is also appreciated for communication and cooperation with materials and other engineering professionals. |
| <u>Prenosljive spretnosti</u> Študent je usposobljen tako za eksperimentalno delo na področju katalitskih procesov kot za strokovno delo pri prenašanju eksperimentalnih rezultatov in literaturnih podatkov v industrijsko prakso. Sposoben je analizirati obstoječe naprave, določiti optimalne pogoje obratovanja in načrtovati nove reaktorje za heterogene reakcijske sisteme. | <u>Skill-transference Ability</u> Developed skills of integrating fundamental chemical and engineering knowledge into processes that are taking place within a multiphase chemical reactor. |

Metode poučevanja in učenja:

Predavanja in seminarji.

Learning and Teaching Methods:

Lectures, seminars.

Delež (v %) /

Načini ocenjevanja:

Weight (in %) **Assessment:**

Pisni in ustni izpit.

Written and oral exam

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, str. 11-24 [COBISS.SI-ID 1752623]

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 [COBISS.SI-ID 36262917]

LIKOZAR, Blaž, **KRAJNC, Matjaž**. Kinetic modeling of the peroxide cross-linking of polymers : from a theoretical model framework to its application for a complex polymer system. Chemical engineering and processing, ISSN 0255-2701. [Print ed.], 2011, vol. 50, no. 2, str. 200-210

[COBISS.SI-ID 35022597],

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 [COBISS.SI-ID 35022341],

KRAJNC, Matjaž, LEVEC, Janez. Oxidation of phenol over a transition-metal oxide catalyst in supercritical water. Industrial & engineering chemistry research, ISSN 0888-5885. [Print ed.], 1997, vol. 36, no. 9, str. 3439-3445 [COBISS.SI-ID 833562]

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