



Univerza v Mariboru

Fakulteta za kemijo  
in kemijsko tehnologijo

**UČNI NAČRT PREDMETA / COURSE SYLLABUS**

<b>Predmet:</b>	Kemijsko računanje II
<b>Course title:</b>	Chemical Calculation II

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Enovit magistrski študijski program druge stopnje Predmetni učitelj	/	2.	Poletni Spring
Five-year master's degree program Spring Subject Teacher	/		

**Vrsta predmeta / Course type**

Izbirni/Elective

**Univerzitetna koda predmeta / University course code:**

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Laboratory work	Teren. vaje Field work	Samost. delo Individ. work	ECTS
20			10		60	3

**Nosilec predmeta / Lecturer:**

doc. dr. Miloš Bogataj

**Jeziki /**

**Predavanja / Lectures:** slovenski/Slovene

**Languages:**

**Vaje / Tutorial:** slovenski/Slovene

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

Anorganska kemija, matematika, računalništvo v kemiji

**Prerequisites:**

Knowledge of inorganic chemistry, mathematics, computer in chemistry.

**Vsebina:****Predavanja:**

- vrste kemijskih procesov (šaržni kontinuirni),
- pretvarjanje enot veličin,
- različni načini reševanja masnih bilanc posameznih procesnih enot (brez in z kemijsko reakcijo),
- sekvenčni in modularni način reševanja masnih bilanc sistemov procesnih enot,
- značilni tokovi v kemijskem procesu (obtok, mimotok, odtok),
- linearna interpolacija in regresija,
- numerično reševanje algebrskih enačb.

**Računalniške vaje:**

Na osnovi osvojene teorije študentje uporabljajo različne načine in orodja pri reševanju masnih bilanc procesnih enot in sistemov procesnih enot. Pri reševanju matematičnih in kemijskih problemov uporabljajo različne numerične metode ter programe, kot so npr: Matlab, Scilab, Python, Excel, Aspen Plus, Polymath.

**Content (Syllabus outline):****Lectures:**

- chemical processes (batch, continuous),
- conversion of units,
- different approaches of solving material balances for single process units (without and with chemical reaction),
- sequential and modular approaches of solving material balances for chemical processes,
- different streams in chemical processes (recycle, bypass, purge),
- linear interpolation and regression,
- solving algebraic equations with numerical methods.

**Computational work:**

On the basis of the learned theory students use different approaches and tools for solving material balances of process units and systems of process units.

They also use different numerical methods and programs such as: Matlab, Scilab, Python, Excel, Aspen Plus, Polymath for solving mathematical and chemical problems.

**Temeljna literatura in viri / Readings:**

- M. Krajnc, S. Oreški, F. Purkeljc, Procesne bilance, Fakulteta za kemijo in kemijsko tehnologijo, Maribor, 2012 (elektronska verzija).
- M. Krajnc, Procesne bilance, zbirka rešenih nalog, zbrano gradivo, FKKT Maribor, 2011 (elektronska verzija).
- S. Oreški, Procesne bilance – računalniške vaje, 2. del, Numerične metode, snovne bilance sistemov brez in s kemijsko reakcijo, FKKT, Maribor, 2007.

Dodatna priporočena literatura:

- R. M. Felder, R. W. Rousseau, Elementary Principles of Chemical Processes, 4th edition, John Wiley & Sons, Inc., New York, ~~2000~~ 2015.
- B. A. Finlayson, Introduction to Chemical Engineering Computing, John Wiley & Sons, Hoboken, New Jersey, 2012

**Cilji in kompetence:**

Sistematično reševanje masnih bilanc v kemijskih procesih, samostojna uporaba programskih paketov Aspen Plus, Polymath in Excel.

**Objectives and competences:**

Systematic solving of material balances in chemical processes, the use of programs Aspen Plus, Polymath and Excel.

**Predvideni študijski rezultati:****Znanje in razumevanje:**

Do rezultatov vodi sistematično reševanje masnih bilanc.

**Intended learning outcomes:****Knowledge and understanding:**

Systematic work leads to the material balances results.

**Prenesljive/ključne spretnosti in drugi atributi:**  
Uporaba komercialnih programov (Aspen Plus, Polymath in Excel) pri podobnih predmetih.

**Transferable/Key Skills and other attributes:**  
The use of commercial programs (Aspen Plus, Polymath and Excel) with similar courses.

**Metode poučevanja in učenja:**  
Aktivno poučevanje in učenje, skupinsko (sodelovalno) delo, e-izobraževanje.

**Learning and teaching methods:**  
Active teaching and learning, cooperative learning, e-learning.

<b>Načini ocenjevanja:</b>	Delež (v %) / Weight (in %)	<b>Assessment:</b>
Izpit je opravljen, če so pozitivno opravljene vse naslednje obveznosti:		Student passes the examination if s(he) successfully passed all the following obligations:
- pisni izpit ali 2 pisna testa,	<b>30</b>	- written test or 2 written tests,
- ustno izpraševanje ali 2 e-testa,	<b>20</b>	- oral examination or 2 e-tests,
- domača naloga,	<b>20</b>	- homework,
- računalniške vaje	<b>30</b>	- computational work.

**Reference nosilca / Lecturer's references:**

- BOGATAJ, Miloš, KRAVANJA, Zdravko. An alternative strategy for global optimization of heat exchanger networks. V: PIERUCCI, Sauro (ur.), KLEMEŠ, Jiri (ur.). PRES 2011, 14th International Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, 8-11 May, 2011, Florence, Italy, (Applied thermal engineering, ISSN 1359-4311, Vol. 43, 2012). [S. l.: s. n.]. 2011, vol. 43, str. 75-90, doi: 10.1016/j.applthermaleng.2011.12.015. [COBISS.SI-ID 15815190]
- KRAVANJA, Zdravko, BOGATAJ, Miloš, SORŠAK, Aleksander. Process integration : HEN synthesis, exergy opportunities. V: PUIGJANER, Luis (ur.). Syngas from waste : emerging technologies, (Green energy and technology (Print), ISSN 1865-3529). London: Springer. cop. 2011, str. 201-225. [COBISS.SI-ID 15630358]
- QUAGLIA, Alberto, PENNATI, Alessandra, BOGATAJ, Miloš, KRAVANJA, Zdravko, SIN, Gürkan, GANI, Rafiqul. Industrial process water treatment and reuse : a framework for synthesis and design. Industrial & engineering chemistry research, ISSN 0888-5885. [Print ed.], 2014, vol. 53, no. 13, str. 5160-5171, doi: 10.1021/ie401379j. [COBISS.SI-ID 17185046] AHMETOVIĆ, Elvis, SULJKANOVIĆ,
- GLAVIČ, Peter, BOGATAJ, Miloš. Water networks - theory and practice. V: ATIMTAY, Aysel T. (ur.), SIKDAR, Subhas K. (ur.). Security of industrial water supply and management : [proceedings of the NATO Advanced Research Workshop on Security of Industrial Water Supply and Management, Ankara, Turkey, 13-15 September, 2010], (NATO science for peace and security series, ISSN 1874-6519, C, Environmental security). Dordrecht: Springer. cop. 2011, str. 13-30. [COBISS.SI-ID