FIŞA DISCIPLINEI

1. Data on the program

1.1 Institution of higher education	Babeş-Bolyai University, Cluj-Napoca
1.2 Faculty	Chemistry and Chemical Engineering
1.3 Department	Chemistry
1.4 Area of study	Chemical Engineering
1.5 Cycle of study	Master
1.6 Study program / qualification	Advanced process engineering, master in chemical engineering

2. Data on the discipline

2.1 Name of the discipline	**Molecular modeling and design CME7331**						
2.2 Lecturer			Conf. dr. Gabriela Nemes				
2.3 Seminar/laboratory assistant			Conf. dr. Gabriela Nemes				
2.4 Year	II	2.5 Semester	3	2.6. Type of evaluation	VP	2.7 Regime of the discipline	**Op**

3. Total estimated time (hours per semester for teaching/learning activities)

3.1 Hours per week	3	Of which: 3.2 course	2	3.3 seminar/laboratory	1
3.4 Total total hours in curriculum	42	Of which: 3.5 course	28	3.6 seminar/laboratory	14
Distribution of time:					ore
Study using manuals, lecture support, bibliography, notes					20
Additional documentation in the library, on electronic databases, on field					20
Preparation of seminaries/laboratories, homework, essays					60
Tutoring					4
Examination					4
others:					-

3.7 Total hours individual study	108
3.8 Total hours per semester	150
3.9 Number of credits	6

4. Preconditions (if existing)

4.1 curriculum	-
4.2 competences	-

5. Conditions (if applicable)

5.1 Lecture	• Mobile phones off or silent • Powerpoint presentations distributed to the students after the course
5.2 Seminar/laboratory	• Mobile phones off or silent • Homework (written and as attached calculation files) to be turned in electronically or printed, on time

6. Specific competences

Professional competences	• Technological design of processes and instruments specific to process engineering for improvement of performance in chemical and biochemical processes unsing computer-aided design (CAD) and sustainable development principles • Development of mathematical models and of simulations in process engineering, for diagnosing problems, analyzing optimal running conditions, and handling of (bio)chemical processes
transverse competences	• Independent completion of complex professional tasks and autonomous conduction of research and design experiments, using computer-aided design and complying with moral and professional ethics standards • Planning, monitoring and endorsement of professional tasks within a hierarchy-bound professional group. Demonstration of abilities to coordinate activities, analytical thinking flexibility, collaboration with team members • Self-evaluation of performance and appraisal of the needs for continuing education, continuing documentation and formation in the respective field of activity and in related fields, in line with the requirements of the labor market

7. Objectives of the discipline

7.1 general objectives	• Familiarize students with basic and advanced notions, concepts, theories and basic models in chemistry and chemical engineering
7.2 specific objectives	• Acquire knowledge for improving the performance of chemical and biochemical processes using computer-aided design and the principles of sustainable development • Acquire knowledge for using and developing mathematical models and simulations in process engineering, for diagnosing problems, analyzing the optimal working regimes for (bio)chemical processes

8. Content

8.1 Lecture	Teaching methods	Observations
8.1.1.Introduction in molecular modeling; definition of the field; relationship with other branches of chemistry	Lecture; explication; conversation; description	
8.1.2.Potential energy surfaces	Lecture; explication; conversation; description	
8.1.3.Molecular mechanics	Lecture; explication; conversation; description	
8.1.4-5.Basis of molecular orbital theory.	Lecture; explication; conversation; description	
8.1.6.Semiempirical MO methods	Lecture; explication; conversation; description	
8.1.7.Ab initio MO methods	Lecture; explication; conversation; description	
8.1.8.Post-HF methods	Lecture; explication; conversation; description	
8.1.9.Density functional theory (DFT).	Lecture; explication; conversation; description	

8.1.10.Hybrid QM/MM methods	Lecture; explication; conversation; description	
8.1.11.Molecular properties calculations	Lecture; explication; conversation; description	
8.1.12.Molecular properties calculations: determination of charge distribution; electrostatic potential surfaces	Lecture; explication; conversation; description	
8.1.13.Excited state calculations	Lecture; explication; conversation; description	
8.1.14.Determination of reaction mechanisms via transition state calculations	Lecture; explication; conversation; description	
Bibliography 1. C.J.Cramer, *Essentials of Computational Chemistry, Theories and Models*, Wiley, 2004. 2. E.Lewars, *Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, Kluwer Academic Publishers, 2003 3. I.Silaghi-Dumitrescu, D. Horvath, *Mecanică Moleculară*, Presa Universitară Cluj-Napoca, 1996. 4. F.Jensen, *Introduction to Computational Chemistry*, Wiley, 1999.		
8.2 Seminar / laboratory	Teaching methods	Observations
8.2.1. Presentation of the seminar topics; conditions, requirements for completing assignments. Introductory notions.	Lecture; explication; conversation; description; experiment	
8.2.2. Building molecular models on the computer	Lecture; explication; conversation; description; experiment	
8.2.3. Modeling molecular shape and energy using molecular mechanics	Lecture; explication; conversation; description; experiment	
8.2.4-5. Modeling molecular shape and energy using ab initio and semiempirical methods	Lecture; explication; conversation; description; experiment	
8.2.6. Modeling complex molecular properties detectable at macroscopic level	Lecture; explication; conversation; description; experiment	
8.2.7-8. Building models involving more than one molecule; supramolecular systems, nanosystems	Lecture; explication; conversation; description; experiment	
8.2.9-10. Modeling chemical reactivity at molecular and supramolecular level	Lecture; explication; conversation; description; experiment	
8.2.11-12. Modeling shape and energy in supramolecular and nano systems	Lecture; explication; conversation; description; experiment	
8.2.13. Dynamics techniques	Lecture; explication; conversation; description; experiment	
8.2.14. Evaluation	Test	
Bibliography 1. W.J. Hehre, A.J. Shusterman, W.W. Huang, *A laboratory Book of Computational Organic Chemistry*, Wavefunction, Irvine, California, 1996. 2. *Spartan '04. Tutorial and User Guide*, Wavefunction, 2003.. 3. Laboratory handouts: https://sites.google.com/site/modelaresidesignmolecular/		

9. Correlating course content with the expectations of the epistemic community representatives, professional associations and employers representative for the program

- By learning the theoretical and methodological concepts and addressing practical aspects included in the outline of the course, students acquire appreciable knowledge, consistent with the partial competencies required for possible occupations provided in Grid 1 - RNCIS.

10. Evaluation

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Weight on final grade
10.4 Course	Correctness of answers – apprehension and comprehension of the issues discussed in the lectures	Written examination – conditioned by completion of the laboratory activities. Attempted fraud is sanctioned by stopping the examination. Fraud is sanctioned by expulsion as per the ECST regulations of BBU	80%
	Correct solving of the problems		
10.5 Seminar/laboratory	Correctness of answers – apprehension and comprehension of the issues discussed in the seminar/laboratory	Grading is based on the completed homework – written as well as in the form of electronic files requested for the modeling activities	20%
	Quality of homework		
	Quality of work during the laboratory/seminar		
10.6. Minimal standards of performance			
• Grade equal to 5 (five). • Knowledge of introductory notions; application of the modeling methods on a material of known chemical composition, identifying those properties which can be predicted and the level of precision/utility of the applied methods			

Date | Signature of lecturer | Signature of seminar/laboratory assistant

25.03.2017

Date of approval by the department

14 aprilie 2017

Signature of department director

Prof. Dr. Cristian SILVESTRU