Subject card

Subject name and code	Modelling in Environmental Protection, PG_00054837					
Field of study	Environmental Protection					
Date of commencement of studies	October 2026		Academic year of realisation of subject		2026/2027	
Education level	Master's studies		Subject group		Obligatory subject group in the field of study Subject group related to scientific research in the field of study	
Mode of study	full-time studies		Mode of delivery		at the university	
Year of study	1		Language of instruction		Polish	
Semester of study	1		ECTS credits		1.0	
Learning profile	academic		Assessment form		credit	
Conducting unit	Laboratory of Environmental Chemoinformatics -> Department of Environmental Chemistry and Radiochemistry -> Faculty of Chemistry -> Rector					
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Tomasz Puzyn				
	Teachers					
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	0.0	0.0	15
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM	
	Number of study hours	15	2.0	8.0	25	
Subject objectives	- Become familiar with the risk assessment of chemicals taking into account the principles of the European REACH system and legal obligations - Become familiar with the possibilities and limitations of computational modeling methods used in environmental risk assessment, with a special focus on QSAR/QSPR and MM models - Become familiar with available software and the possibilities of using tools in the process of chemical risk assessment - To develop the ability to independently plan and carry out elements of chemical risk assessment on the basis of modelling methods					

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[OŚMU2_K08] Initiates and takes into account in the organizational activity the activities for the social environment and public interest.	After completing the course, each student will: 1. recognise the need to carry out risk assessments of newly designed chemical compounds in a social context (improving the quality of life of society); 2. be able to participate in the discussion of modern environmental problems based on sound scientific arguments; 3. understands the need for further training; demonstrates the most independent, active approach to problems and creativity in both individual and team work;	[SK8] observation of student's independent or team work
	[OŚMU2_U04] Critically analyses experimental data on environmental protection by statistical methods and modelling using IT techniques and tools.	After completing the course, each student will: 1. be able to give examples of the use of physical and mathematical models in modern environmental protection; 2. relate the chemical properties of a compound to its fate in the natural environment; 3. uses available QSPR models (EPI-Suite, PBT Profiler) to determine the physical and chemical properties of a compound; 4. uses available MM models (OECD tool) to determine the overall persistence and the potential for diffusion of a chemical compound in the environment; 5. critically review the modelling results obtained; be able to improve the preparation of a report on the research carried out with particular attention to three elements: (i) presentation of the results, (ii) discussion of the results obtained and (iii) correct formulation of the conclusions of the modelling carried out.	[SU8] observation of student's independent or team work
	[OŚMU2_W04] Chooses methods, techniques and research tools used in environmental protection.	After completing the course, each student will be able to 1. recognise the advantages and disadvantages of using models in environmental risk assessment; understand the principles of REACH in Europe and the legal obligations arising from it; 2. know the main theories describing the processes of regional and global dispersion of chemical pollutants and the basic physical and chemical laws on which these theories are based; 3. know the process of building and validating the QSAR model according to the OECD recommendations 4. know the process of construction and validation of the MM model according to OECD recommendations 5. know the principles of presenting the results of the model studies carried out.	[SW4] test/exam - oral or written

	Course outcome	Subject outcome	Method of verification
	[OŚMU2_W02] Has the thorough knowledge of statistical methods and modeling in environmental protection.	After completing the course, each student will be able to 1. recognise the advantages and disadvantages of using models in environmental risk assessment; understand the principles of REACH in Europe and the legal obligations arising from it; 2. know the main theories describing the processes of regional and global dispersion of chemical pollutants and the basic physical and chemical laws on which these theories are based; 3. know the process of building and validating the QSAR model according to the OECD recommendations 4. know the process of construction and validation of the MM model according to OECD recommendations 5. know the principles of presenting the results of the model studies carried out.	[SW4] test/exam - oral or written
Subject contents	A. The problems of the lecture:1. Models and modelling: concept of model; basic classification of models (physical and mathematical); examples of models used in environmental protection; advantages and limitations of models.2. Problems of environmental pollution by chemical substances: accidents related to the uncontrolled release of chemical substances into the environment; history of environmental protection by chemical substances; sources of chemical pollution and overview of the main substances considered hazardous; national and international strategies and regulations in the field of environmental protection by chemical substances (including the REACH Regulation); basic assumptions of risk. REACH Regulation); basic assumptions of the risk assessment of chemical pollutants; physical and chemical properties of a compound that are of key importance for chemical risk assessment; processes of the distribution of chemical compounds in the environment; persistence and degradation of chemical compounds; bioaccumulation and biomagnification phenomena in trophic networks; the concept of toxicity and types of toxic effects; chemical compounds identified by the acronyms PBT and vPvB.3. Quantitative structure-activity relationships (QSARs) and quantitative structure-property relationships (QSPRs) as examples of mathematical probabilistic models used in the risk assessment of chemical compounds. Quantitative Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) as examples of mathematical probabilistic models used in the risk assessment of chemical compounds: the idea of QSAR/QSPR modelling; chemical structure decryptors; quality assessment of available experimental data used in modelling; construction and validation of QSAR/QSPR models; available models applicable to chemical risk assessment (EPI-Suite, PBT Profiler).4. Multicomponent environmental mass balance models of chemical pollutants as examples of mathematical deterministic models: concept of multicomponent environmental models; applications of multicomponent models; levels of complexity and sub-assumptions of different types of models; model inputs and their sources; examples of commonly used multicomponent models; idea of modelling based on a combination of QSPR-MM techniques; exposure scenario building based on computational modelling.		
Prerequisites and co-requisites	1. basic computer skills (copying files and running applications in Windows/Linux operating system, spreadsheet, web browser)2. knowledge and skills in physical chemistry, environmental law and toxicology within the scope of the undergraduate curriculum;3. knowledge of English at level B2 of the Common European Framework of Reference for Languages.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	exam	51.0%	100.0%

Recommended reading	Basic literature	Rozporządzenie (WE) nr 1907/2006 Parlamentu Europejskiego i Rady z dnia 18 grudnia 2006 r. w sprawie rejestracji, oceny, udzielaniazezwoleń i stosowanych ograniczeń w zakresie chemikaliów (REACH) i utworzenia Europejskiej Agencji Chemikaliów, zmieniające dyrektywę1999/45/WE oraz uchylające rozporządzenie Rady (EWG) nr 793/93 i rozporządzenie Komisji (WE) nr 1488/94, jak również dyrektywę Rady76/769/EWG i dyrektywy Komisji 91/155/EWG, 93/67/EWG, 93/105/WE i 2000/21/WE.UN-ECE 1998: Protocol to the 1979 convention on long range transboundary air pollution on persistent organic pollutants and executive bodydecision 1998/2 on information to be submitted and the procedure for adding substances to annexes I, II or III to the protocol on persistentModelowanie w ochronie środowiska #7.2.0599 | Strona 3 z 5Modelowanie w ochronie środowiska #7.2.0599Sylabusy - Centrum Informatyczne UGDział Kształceniaorganic pollutants. Document: ECE/EB.AIR/60, United Nations, New York, Geneva.UNEP 2001: Final act of the conference of plenipotentiaries on the Stockholm convention on persistent organic pollutants. Document:UNEP/POPS/CONF/4., United Nations Environment Programme, Stockholm.T. Puzyn, J. Leszczynski, M. T. D. Cronin: Recent Advances in QSAR Studies: Methods and Applications. ?Springer (2010). ISBN: 978-1-4020-9782-9.The OECD software tool for screening chemicals for persistence?and long-range transport potential?Fabio Wegmann, Laurent Cavin, MatthewMacLeod, Martin Scheringer, Konrad Hungerbuhler Environmental Modelling & Software 24 (2009) 228237.OECD 2002: Report of the OECD/UNEP Workshop on the Use of Multimedia Models for Estimation Overall Environmental Persistence andLong-Range Transport in the context of PBTs/POPs Assessment, OECD Environment, Health and Safety Publications, Paris, France.OECD 2004: Guidance Document on the Use of Multimedia Models for Estimatig Overall Environmental Persistence and Long-Range Transprt,OECD Environment, Health and Safety Publications, Paris, France.Puzyn T., Mostrąg A., Suzuki N., Falandysz J. QSPR-based estimation of the atmospheric persistence for chloronaph-thalene congeners. Atmos.Environ. 42 (2008) 6627-6636.
	Supplementary literature	*Falandysz J. (1999): Polichlorowane bifenyle (PCBs) w środowisku: chemia, analiza, toksyczność, stężenia i ocena ryzyka. Fundacja Rozwoju* *Uniwersytetu Gdańskiego, Gdańsk.* *Klasmeier J., Matthies M., Macleod M., Fenner K., Scheringer M., Stroebe M., Le Gall A. C., McKone T., Van De Meent D., Wania F. (2006):* *Application of multimedia models for screening assessment of long-range transport potential and overall persistence. Environ. Sci. Technol. 40,* *53-60.* *Wania F., Mackay D. (1995): A Global Distribution Model for Persistent Organic-Chemicals. Sci. Total Environ. 160-61, 211-232.* *Gouin T., Mackay D., Jones K. C., Harner T., Meijer S. N. (2004): Evidence for the "grasshopper" effect and fractionation during long-range* *atmospheric transport of organic contaminants. Environ. Pollut. 128, 139-148.*
	eResources addresses	

Example issues/ example questions/ tasks being completed	brak
Work placement	Not applicable

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