

Subject card

Subject name and code	Modelling in Environmental Protection, PG_00054838						
Field of study	Environmental Protection						
Date of commencement of studies	October 2024	Academic year of realisation of subject			2024/2025		
Education level	postgraduate studies	Subject group			Obligatory subject group 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					
Conducting unit	Pracownia Analityki i Radiochemii Środowiska -> Katedra Chemii i Radiochemii Środowiska -> Faculty of Chemistry						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Tomasz Puzyn				
	Teachers		mgr inż. Natalia Buławska				
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	15.0	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	The objective of this course is to familiarise students with the basic environmental issues and risk assessment of chemical compounds. In addition, the course introduces and applies examples of tools used in risk assessment. Furthermore, the course aims to familiarise students with the benefits and limitations of the programmes/tools used.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[OŚMU2_W04] Chooses methods, techniques and research tools used in environmental protection.	By acquiring an understanding of the range of available methods, tools, and softwares for environmental modelling, the researcher is able to select the most appropriate solution in terms of its suitability, time-efficiency, cost-effectiveness and applicability to the topic of the research problem.	[SW3] text preparation/written work
	[OŚMU2_U04] Critically analyses experimental data on environmental protection by statistical methods and modelling using IT techniques and tools.	Student is able to evaluate the quality of the experimental data used and of the data predicted by means of informatic tools. Furthermore, is able to carry out statistical and comparative analyses of the results obtained on the basis of appropriate research protocols.	[SU3] text preparation/written work
	[OŚMU2_K08] Initiates and takes into account in the organizational activity the activities for the social environment and public interest.	The student should become familiar with the benefits of using the methods presented during laboratory classes. Demonstrates an awareness of the advantages of responsible risk assessment.	[SK3] text preparation/written work
[OŚMU2_W02] Hypothesises and analyses the results using statistical methods and modelling in environmental protection.	Demonstrates an understanding of the fundamental statistical techniques employed in the examination of environmental data. The individual in question employs elementary mathematical formulae to estimate the contents of chemicals in various environmental elements (eg. water, soil, and air).	[SW3] text preparation/written work	
Subject contents	<ol style="list-style-type: none"> 1. The most important physicochemical properties affecting the persistence and dispersion of chemical compounds in the environment; preparation of a full risk characterisation of selected chemicals. 2. Quantitative structure-property relationship modelling (QSPR) for new chemical compounds; critical evaluation of the results obtained; correct preparation of a report on the research carried out with particular emphasis on 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; copyright protection issues. 3. Modelling of total persistence and mobility of tested compounds in the environment based on multicomponent (MM) models; critical assessment of the obtained results; correct preparation of a report on the conducted research with particular emphasis on 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; copyright protection issues. 		
Prerequisites and co-requisites	<ul style="list-style-type: none"> • basic computer skills, including the ability to copy files and run application on Windows/Linux, as well as a working knowledge of spreadsheet and web browser software; • knowledge in the topic of physical chemistry, environmental law, and toxicology within the context of the Bachelor's degree programme; • English at the B2 level of the Common European Framework of Reference for Languages (CEFR). 		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	raport, oral answer	50.0%	100.0%

Recommended reading	Basic literature	<ul style="list-style-type: none"> • Script and instructions for exercises prepared by teacher. • Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC • UN-ECE 1998: Protocol to the 1979 convention on long range transboundary air pollution on persistent organic pollutants and executive body decision 1998/2 on information to be submitted and the procedure for adding substances to annexes I, II or III to the protocol on persistent organic 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, Matthew • MacLeod, Martin Scheringer, Konrad Hungerbühler Environmental Modelling & Software 24 (2009) 228-237. • OECD 2002: Report of the OECD/UNEP Workshop on the Use of Multimedia Models for Estimation Overall Environmental Persistence and Long-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 Estimating Overall Environmental Persistence and Long-Range Transport, OECD Environment, Health and Safety Publications, Paris, France. • Puzyn T., Mostrag A., Suzuki N., Falandysz J. QSPR-based estimation of the atmospheric persistence for chloronaphthalene congeners. Atmos. Environ. 42 (2008) 6627-6636.
	Supplementary literature	<ul style="list-style-type: none"> • 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	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	<ul style="list-style-type: none"> • mathematical calculations related to the spread of chemical compounds in the environment, including the use of developed equations and the conversion of units. Students will be expected to draw appropriate conclusions based on the results obtained. • make predictions based on the developed QSPR model; introduce students to the OECD principles of model development, as well as the steps involved in optimising a molecule and calculating descriptors. Independent student work will include searching databases. Students will be expected to undertake statistical analysis and visualisation of results obtained and to form appropriate final conclusions. • the utilisation of available tools, such as <i>SimpleBox</i>, to simulate the fate of chemical compounds in the environment. 	

Document generated electronically. Does not require a seal or signature.