REVIEW
of the official reviewer for dissertation work
of Mrs. Anel Kapar on the theme «Modeling of solid-phase microextraction of volatile organic compounds from environmental objects» presented for the degree of Doctor of Philosophy (PhD) in the specialty «8D05301 - Chemistry».

№	Criteria	Eligibility (one of the options must be checked)	Justification of the position of the official reviewer
1.	The topic of the thesis (as of the date of its approval) corresponds to the directions of development of science and/or state programs	1.1 Compliance with priority areas of science development or government programs:	Thesis was completed within the framework of project AP08052684 'Effective development of methods for analyzing environmental objects based on headspace solid-phase microextraction using computer modeling' (2020-2022) and Ph.D. scholarship both funded by the Ministry of Education and Science of Republic of Kazakhstan
		1) The thesis was completed within the framework of a project or target program financed from the state budget (indicate the name and number of the project or program) 2) The thesis was completed within the framework of another state program (indicate the name of the program) 3) The dissertation corresponds to the priority direction of the development of science, approved by the Higher Scientific and Technical Commission under the Government of the Republic of Kazakhstan (indicate the direction)	
2.	Importance for science	The work makes/does not make a significant contribution to science, and its importance is well disclosed/not disclosed	The research conducted in the framework of Ph.D. thesis of Ms. Anel Kapar is valuable and its contribution was well presented. Computational methods for research of the process of solid-phase

			microextraction (SPME) possess numerous advantages such as deeper understanding of extraction processes, decreasing costly, time-consuming and laborious experiments of optimization of parameters. Furthermore, development of SPME methods in research of environmental pollution contributes to efficient monitoring of hazardous compounds, thus decreasing economic losses and allowing the assessment and reduction of the effect of pollution on public health
3.	The principle of independence	Self-reliance level: 1) High; 2) Medium; 3) Low; 4) No independence	According to presented articles, reviews of the work by scientific supervisors and credit authorship taxonomy, the contribution of the Ph.D. candidate to presented work was major. The candidate is also a first author in one of the articles (Q1 quartile), and second author in two articles presented for defense
4.	The principle of inner unity	4.1 Justification of the relevance of the thesis: 1) Justified; 2) Partially justified; 3) Not justified.	The relevance of the topic was well justified in the thesis (introduction) and research papers (introduction and discussion)

		4.2 The content of the thesis reflects the topic of the thesis: 1) Reflects; 2) Partially reflects; 3) Does not reflect	All chapters of thesis were dedicated to modeling of solid-phase microextraction of BTEX compounds from samples of air, water and soil, as indicated in the topic
		4.3. The purpose and objectives correspond to the topic of the thesis: 1) correspond; 2) partially correspond; 3) do not correspond	
		4.4 All sections and provisions of the thesis are logically interconnected: 1) completely interconnected; 2) the interconnection is partial; 3) there is no interconnection	
		4.5 The new solutions (principles, methods) proposed by the author are reasoned and evaluated in comparison with the known solutions: 1) there is a critical analysis; 2) partial analysis; 3) the analysis does not represent one's own opinions, but quotes from other authors	Critical analysis of applied methods for determination of diffusion coefficients of analytes was carried out as compared to models with application of other methods referring to relative standard deviation values, when comparing to experiment
5.	Scientific novelty principle	5.1 Are the scientific results and provisions new? 1) completely new; 2) partially new (25-75% are new); 3) not new (less than 25% are new)	Scientific results and provisions are novel and were not reported previously elsewhere
		5.2 Are the dissertation findings new? 1) completely new; 2) partially new (25-75% are new); 3) not new (less than 25% are new)	

		5.3 Technical, technological, economic or management decisions are new and reasonable: 1) completely new; 2) partially new (25-75% are new); 3) not new (less than 25% are new)	
6.	The validity of the main findings	All main conclusions are/are not based on scientifically significant evidence or well-grounded (for qualitative research and areas of training in the arts and humanities)	
7.	The main provisions for the defense	It is necessary to answer the following questions for each provision separately: 7.1 *Provision 1:* Is the provision proven? 1) proven; 2) rather proven; 3) rather not proven; 4) not proven 7.2 Is it trivial? 1) yes; 2) no 7.3 Is it new? 1) yes; 2) no 7.4 Application level: 1) narrow; 2) medium; 3) wide 7.5 Is it proven in the article? 1) yes; 2) no *Provision 2:* Is the provision proven? 1) proven;	

		2) rather proven; 3) rather not proven; 4) not proven 7.2 Is it trivial? 1) yes; <u>2) no</u> 7.3 Is it new? <u>1) yes;</u> 2) no 7.4 Application level: 1) narrow; <u>2) medium;</u> 3) wide 7.5 Is it proven in the article? <u>1) yes;</u> 2) no *Provision 3:* Is the provision proven? <u>1) proven;</u> 2) rather proven; 3) rather not proven; 4) not proven 7.2 Is it trivial? 1) yes; <u>2) no</u> 7.3 Is it new? <u>1) yes;</u> 2) no 7.4 Application level: 1) narrow; <u>2) medium;</u> 3) wide 7.5 Is it proven in the article?	

		1) yes; 2) no *Provision 4:* Is the provision proven? 1) proven; 2) rather proven; 3) rather not proven; 4) not proven 7.2 Is it trivial? 1) yes; 2) no 7.3 Is it new? 1) yes; 2) no 7.4 Application level: 1) narrow; 2) medium; 3) wide 7.5 Is it proven in the article? 1) yes; 2) no *Provision 5:* Is the provision proven? 1) proven; 2) rather proven; 3) rather not proven; 4) not proven 7.2 Is it trivial? 1) yes; 2) no 7.3 Is it new? 1) yes; 2) no	

		7.4 Application level: 1) narrow; 2) medium; 3) wide 7.5 Is it proven in the article? 1) yes; 2) no	
8.	The principle of reliability Reliability of sources and information provided	8.1 Choice of methodology - is justified or the methodology is described in sufficient detail 1) yes; 2) no	Methodology was described in sufficient detail, allowing repeating the experiments. Development of novel experimental design to verify modeling results is innovative and a significant advantage of the thesis
		8.2 The results of the thesis were obtained using modern methods of scientific research and methods of processing and interpreting data using computer technologies: 1) yes; 2) no	The research was carried out with application of modern modeling software such as COMSOL Multiphysics, and experimental data for verification of the models was collected using gas chromatography-mass spectrometry
		8.3 Theoretical conclusions, models, identified relationships and patterns have been proven and confirmed by experimental research (for areas of training in pedagogical sciences, the results have been proven on the basis of a pedagogical experiment): 1) yes; 2) no	Models and theoretical conclusions were proven and confirmed by experimental data with the RSD values < 15%

		8.4 Important statements are confirmed/partially confirmed/not confirmed by references to current and reliable scientific literature	Current and reliable scientific literature were included to confirm important statements, including coefficients for performing simulations, structure of porous coatings, critical analysis of methods used for determination of molecular descriptors for modeling
		8.5 Used literature sources are sufficient/not sufficient for a literature review	
9	Practical value principle	9.1 The thesis has theoretical value: 1) yes; 2) no	Thesis has both theoretical and practical value, providing insights into SPME process, which is in all cases advantageous for users. In addition, models can be applied for optimization of extraction parameters
		9.2 The thesis is of practical importance and there is a high probability of applying the results obtained in practice: 1) yes; 2) no	Developed models can be used in future for modeling of extraction process, and optimize extraction parameters without experiments
		9.3 Are the practice suggestions new? 1) completely new; 2) partially new (25-75% are new); 3) not new (less than 25% are new)	
10.	The quality of writing and design	Academic writing quality: 1) high; 2) average; 3) below average; 4) low.	All scientific terminology was used correctly. Scientific writing was performed at academic level, no significant errors and redundant text were observed. The sentences are logically connected, and their meaning is clear and readable

11.	Notes on a thesis	The volume of the research work that was carried out in the framework of Ph.D. study is significant, which indicates that the Ph.D. candidate spent a sufficient amount of time dedicated to research, and not only achieved the main goal and fulfilled the tasks of the work, but also performed a contribution to science. The goal of the work is innovative and unconventional, which is also a significant advantage of presented results. It could be interesting to study in the future how three-dimensional conformation of molecules of analytes affect their adsorption into the pores, considering their depth and shape, and if it could be considered in computational models. On the other hand, possibly this factor does not affect the precision of the models or is already considered in the adsorption isotherm. This comment has been made only for scientific discussion and does not affect the assessment of the thesis, which was performed at high quality.	
12.	Scientific level of the doctoral student's articles on the topic of research (in case of defense of the dissertation in the form of a series of articles, the official reviewers comment on the scientific level of each article of the doctoral student on the topic of research)		
13.	Decision of the official reviewer (pursuant to paragraph 28 of the present Model Regulations)	to award the degree of Doctor of Philosophy (PhD) or Doctor of Specialization	The presented work demonstrates high scientific quality. The findings are novel and make valuable contributions to science. The modeling of the extraction process demands a strong theoretical foundation, reflecting

			the candidate's strong educational background and high level of qualification. The candidate has exhibited a high level of independence, possessing well-developed research skills and knowledge, and is well-prepared to embark on a research career

Official Reviewer:

Postdoctoral researcher at the University of Tubingen, PhD  Gulyaim Sagandykova