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REVIEW

regarding the defense of a PhD thesis on the topic: CFD MODELING OF MEMBRANE SEPARATION THROUGH NANOFILTRATION"

for the acquisition of: educational and scientific degree "doctor"

in the specialty – "Processes and devices in chemical and biochemical technology"

with candidate - Eng. Stella Plamenova Panyovska

Reviewer/ Tatyana Stefanova Petrova, PhD, professor

- **Brief biographical data and a description of the scientific interests and scientific activities of the PhD candidate.**

PhD student Stella Panyovska graduated from the University of Chemical Technology and Metallurgy - Sofia, CAD/CAE in chemical technology in 2017, professional qualification - chemical engineer, with an excellent overall grade point average (5.50) from her studies and a grade from the defense of her master thesis "3D design and analysis of a reactor with mechanical stirring and aeration" - with an excellent grade (6.00). She started working at the Institute of Chemical Engineering at the Bulgarian Academy of Sciences (IChE-BAS) even before she officially graduated, as a chemist from 01.03.2017 to 23.02.2022; then she was appointed as an assistant in the Laboratory "Transport Processes in Multiphase Media" at IChE-BAS. Since 2020, she is enrolled in PhD studies for individual training preparation with scientific advisors Assoc. Prof. Dr. Daniela Djonova (current professor) and Prof. Dr. Iren Tsibranska, and the working title of the PhD thesis is "CFD modeling of membrane separation by nanofiltration". According to the Regulations of the Educational Centre for PhD students of the Bulgarian Academy of Sciences and according to the decision of the Colloquium of Scientists at the IChE of 29.09.23, Eng. Panyovska has covered and exceeded the required credit points according to the plan for her PhD studies (441 from 250 required) and has fulfilled the internal requirements at the IChE with the right to defense. She was deducted with the right to defense by order RD 15-518/27.10.23. On 27.11.25, The IChE Colloquium reviewed her dissertation work at the pre-defense and directed it to defense; this decision was approved at a meeting of the National Council of the Institute of Chemical Engineering with Protokol No. 10/04.12.2025.

The PhD student's scientific interests are in the field of chemical engineering, in general - in the experimental and theoretical study of extraction, distillation, absorption, adsorption processes in reactors. Her specific scientific competence and skills are manifested in the field of computational fluid dynamics (CFD), 3D design and simulation of stirred and aerated reactors, airlift reactors, bell-tray columns, etc., a topic covered in her master's

thesis.

Her scientific assets, according to the submitted documents, are expressed in a total of 14 publications (10 of them in scientific journals with SJR/IF), 33 citations to them, participation in 6 projects at the National Science Foundation (5 completed, 1 ongoing), 2 participations as a young scientist in the National Research Programm "Young Scientists and Postdoctoral Fellows" - sessions 2019 and 2022. The doctoral student's scientific achievements were honored in 2021 with the award of the BAS Prize in the competition for the youngest scientists under 30 years old "Ivan Evstratiev Geshov", in the scientific field "Energy Resources and Energy Efficiency".

- **Relevance of the problem developed in the dissertation.**

Nanofiltration as a membrane separation process and the membrane reactors in which it is carried out is a current scientific topic, which, after its emergence in the 1980s, continues to develop and finds more and more new applications in various branches of industry (drinking water production, wastewater treatment, food industry, chemical and pharmaceutical industries, etc.). The chosen topic of the PhD thesis (PhDT) is definitely relevant and significant; this is also confirmed by the literature review in the PhDT - the growth of research in the field of nanofiltration is so rapid that more than two-thirds of the total publications in this area have been published in the last decade. Significant and current issues in the membrane filtration that are currently facing the global scientific community include reducing/preventing membrane fouling and assessing the efficiency of the mass transfer rate across the membrane surface. The presented PhDT proposes solutions to the above problems using CFD as a useful theoretical tool that can provide new knowledge about the velocity distribution around and along the membrane surface, as well as for assessing mass transfer and its efficiency in the membrane nanofiltration.

- **Review of the dissertation work and analysis of the results.**

The presented PhDT (total 151 pages) is organized into 7 chapters, contains 62 figures, 2 tables and 169 cited literature sources; also, there are included an introduction, a description of the used notations and abbreviations, as well as the lists of publications and reports of scientific results on the topic of PhDT. Of the cited literature, 159 sources are after 2000, 6 sources before 2000 and 4 are without a specific year of publication. The selection and analysis of the literary sources in Chapter I (literary review, 35 pages) speaks of a very complete and precise approach to the collection, presentation and summary of useful information and contemporary data on the topic of PhDT. The review examines in detail the main issues - what is nanofiltration, the types of nanofiltration membranes and the materials from which they are made, their use in the integrated membrane reactors and their applications. A description of the scientific trends in theoretical research on the nanofiltration membranes is also made, as the PhD student has

correctly emphasized and described the published and achieved results on the topic using CFD. Examples of the use of CFD in studying the different approaches to membrane modeling, for optimizing the hydrodynamics of membrane reactors and membrane modules in single and multiphase flows, in flows with different rheology, etc., as well as for assessing mass transfer and efficiency in the relevant membrane processes, are considered. The conclusions from Chapter I are clearly formulated in Chapter II (2 pages) and show the need for the research conducted in the PhDT; from them naturally arise the PhD's thesis goal and the tasks set (Chapter III, 2 pages).

The purpose and tasks of the PhDT are correctly defined and clearly explained. The formulated tasks are 6, as follows: 1) Modeling the hydrodynamics of filtration cells with membrane modules, by applying computerized CFD methodology; 2) Determination of shear stresses, dynamic pressure and hydrodynamic mixing regimes, depending on the specifics of the particular system; 3) Analysis of the available correlations for mass transfer coefficients near the semi-permeable membrane, as well as those predicted by CFD simulations; 4) Study of mass transfer in different designs of nanofiltration cells: in the boundary layer to the membrane surface, for the cell as a whole and determination of mass transfer coefficients from the fluid to the membrane; 5) A method will be proposed for assessing the efficiency of the filtration process through key parameters that link hydrodynamics with the separation process in order to determine the optimal process conditions; 6) Comparison of CFD simulations with experimental data. The PhD student has presented two working hypotheses for the hydrodynamic and mass transfer part in the research tasks set; the objects of the study are 3 types of filtration cells (FC) with different shapes and with different ways of supplying the permeate flow (with a mixer, tangential and cross). I believe that a sufficiently wide scope and diversity of the objects is provided in the research tasks set in the PhDT.

Chapter IV (24 pages) presents a detailed description of the CFD algorithm (formulation, geometric model, meshing, iterative procedure for obtaining the solution, analysis) and the types of models that can be used to study the hydrodynamics under different flow regimes and to determine the mass transfer coefficient through the membrane. It is also explained how the mass transfer coefficient (Reiss-Hanratty equation) will be calculated from the obtained numerical hydrodynamic results for the distribution of local velocities and shear stresses. The PhD student also proposed a new approach for assessing the efficiency of mass transfer in a membrane during filtration based on the obtained numerical solutions.

Chapter V (47 pages) describes and analyzes the obtained numerical results using the CFD methodology for the three types of studied FC in PhDT: 1) Dead-End FC with a mixer and a flat bottom membrane; 2) Cross-Flow (CF) FC - circular with tangential fluid supply, and 3) Cross-Flow rectangular FC. In two of the studied FCs, the hydrodynamic regime is turbulent, and in the third - laminar; to model the turbulent regime, a

"Realizable k-ε" model was added to the RANS Navier-Stokes equations. For each of the studied FCs, the correct boundary conditions in the meshed geometric models of the FC were determined, as well as the initial values and the convergence criterion for the variables (velocity, turbulent kinetic energy and turbulent kinetic energy dissipation rate), in the iteration procedure. The PhD student also performed the necessary tests for the independence of the results from the mesh, and a good compromise was found between the computational time and the deviations of the parameters.

In the modeling for each FC, preliminary information and data from physical experiments were used (without the personal participation of the PhD student) - for filtration of polyphenols and flavonoids from ethanol extracts of plant raw materials, as well as sugars and phenols from aqueous solutions of plants, in order to correctly and realistically determine the conditions of the simulations. Numerical results were obtained for each of the studied FC for the distribution of velocitiess, shear stresses and mass transfer coefficients, which are presented by a sufficient number of figures. For the DE FC, the influence of the mixer revolutions and the influence of its diameter on the distribution of shear stresses and, respectively, on the mass transfer coefficient, was studied. For the circle CF FC, the influence of the feed flow velocity on the same quantities was studied, and simulations were made for the thickness of the concentration boundary layer depending on different Reynolds numbers at a fixed value of Sc. For the rectangular CF FC, the influence of the feed tangential flow rate on the shear stresses has been studied.

A successful comparison of the obtained results with the available literature data has been made. For the DE FC, the average shear stresses have been compared with experimental data obtained by electrochemical method. For the circle CF FC, the mass transfer coefficient has been compared with respective experimental and model data from two different sources. For the CF rectangular FC, a qualitative confirmation of the obtained results for the velocity distribution and the homogeneity of the shear stress field around the membrane surface has been shown, with data from experimental observations of filtration of sugars and phenols from aqueous extracts of Eurasian water milfoi. The comparisons made confirm the validity of the numerical results obtained in PhDT and the ability of the chosen approach to predict the hydrodynamic picture and the mass transfer coefficient for different FCs (I mean the geometry and the method of flow delivery) and for different hydrodynamic regimes. The same chapter also presents a comparative analysis of the results of CFD simulation of nanofiltration in DE and CF filtration regimes; the new approach for assessing the efficiency of nanofiltration in both FCs is also applied.

Chapter VI (2 pages) presents the contributions of PhDT, which are divided into three groups, as follows: 1) Assessment of the influence of the hydrodynamic picture and distribution of shear stresses in membrane filtration processes using CFD (2 contributions); 2) Description and prediction of mass transfer in membrane filtration

processes using CFD (2 contributions) and 3) Method for assessing membrane efficiency (1 contribution).

Chapter 7 (26 pages) describes in detail and with an accurate bibliography the cited literature sources. I highly appreciate the links (references) to each of them, this allows quick verification and correctness when checking each source. I must also note and appreciate the internal references in the PhDT prepared by the PhD student from the content of the electronic version of the PhDT and in general the way the entire text is laid out, as well as the quality of the figures.

• Main scientific and applied scientific contributions.

It is evident that the PhDT is the personal work of the PhD student eng. Panyovska in all its parts listed above; the same applies to the presented abstract of the PhDT. The abstract correctly describes the main results presented in the PhDT. The main results in the PhDT were obtained independently by the PhD student and show her competence in the modeling of nanofiltration membrane processes using CFD; a guarantee for this is her previous experience and the scientific asset presented to date. I agree with the contributions presented in Chapter VI and their structuring into three different groups. In general, I would define the contributions as scientific - obtaining new theoretical knowledge through CFD, for the hydrodynamic picture and distribution of shear stresses, as well as for predicting mass transfer in membrane filtration processes. I would define the method for assessing membrane efficiency as scientific and applied.

• Description and evaluation of the submitted materials:

I was provided with all necessary documents (in paper and electronic format) for the procedure for the defense of this PhD thesis, as follows: PhDT, abstract (in Bulgarian and English), CV, list and full text of publications included in the thesis – 4 issues, all in English, 2 with SJR and 1 with IF(Q1), report and copies of protocols for the exams taken by the PhD student, report on the fulfillment of the requirements and the credits obtained according to the Regulations of the Centre of education of PhD Students at the Bulgarian Academy of Sciences. A certified report on the absence of plagiarism for the text in the thesis is also attached. The results in the thesis have been reported at 8 conferences, of which 2 abroad. All necessary quantitative criteria have been met and exceeded: a) the minimum requirements for acquiring the ESD "Doctor" in professional field (PF) 4.2 "Chemical Sciences" have been met, according to the Regulations of the Centre of education of the Bulgarian Academy of Sciences for PhD students (441 points out of the mandatory 250 have been collected), and b) the additional requirements of the IChE-BAS for acquiring the ESD "Doctor" have been met, according to the Methodology for the Growth of Scientists at the IChE-BAS, Appendix 1 (55 out of the mandatory 30 points).

• Reflection of the candidate's scientific publications in Bulgarian and foreign

literature.

The publications presented by the doctoral student have been cited 33 times according to the materials presented by her, which clearly shows that her research is highly valued by the scientific community.

• Critical notes and recommendations for the candidate's scientific works.

I have no significant remarks. There are several duplications of notations (p. 5), omitted and incorrectly written indices or quantities in the text (p. 21, 55, 57, 93). I would combine conclusions 2 and 3 of Chapter I. The remarks made are mainly of a technical nature and do not affect my positive opinion of the presented PhDT.

• Personal impressions of the reviewer about the candidate.

I have known Stella Panyovska since she came to IIH. I have very good impressions of her scientific work and her personal qualities.

CONCLUSION

Based on the above, I believe that the candidate for the procedure for acquiring the ESD "Doctor" in the specialty: "Processes and Apparatus in Chemical and Biochemical Technology", PF "4.2. Chemical Sciences" at IChE-BAS, MSc.Eng. Stela Plamenova Panyovska, fully satisfies and covers the requirements of the Regulations on the Terms and Procedure for Acquiring Scientific Degrees and Holding Academic Positions at BAS, as well as the additional requirements of IChE-BAS for acquiring the ESD "Doctor". Based on my positive opinion of the candidate's PhDT, abstract, publications to the PhDT, their significance and the contributions contained therein:

I propose to the esteemed jury to vote positively on the following proposal for a decision: " MSc. Eng. Stella Plamenova Panyovska from the Institute of Chemical Engineering - BAS, to be awarded the ESD "Doctor" in PF 4.2 Chemical Sciences, specialty "Processes and Apparatus in the Chemical and Biochemical Industry".

Date:

14.01.2026

Reviewer:

/prof. Dr. Tatyana Stefanova Petrova, IChE-BAS/