REVIEW

on the competition for the occupation of the Academic position "Professor" in professional field "4.2. Chemical Sciences" with a speciality "Processes and Apparatuses for Chemical and Biochemical Technology" for the needs of the Laboratory "Transfer Processes in Multiphase Media" at the Institute of Chemical Engineering, BAS,

Announced in the State Gazette no. 77 on 10.09.2024

with candidate Assoc. Prof. Dr. Tatyana Stefanova Petrova

Reviewer: Prof. Dr. Sonia Stoyanova Tabakova, Prof. Emeritus at the Institute of Mechanics, BAS

Only one candidate: Associate Professor Dr. Tatyana Stefanova Petrova participates in the competition for the academic position "Professor", who is Associate Professor at the Institute of Chemical Engineering (IChE), BAS. The candidate presented all the required documents according to the law on the Development of the Academic Staff in the Republic of Bulgaria and its implementation in the Institute of Chemical Engineering.

1. Brief scientific biography of the candidate and area of scientific interests

Assoc. prof. Tatyana Petrova is born on 1.10.1966 in Harkov, Ukraine. In 1989 she received her master's degree in Mathematics with a speciality in "Fluid Mechanics" from Sofia University (SU), "St. Clement Ohridski", Faculty of Mathematics and Mechanics (FMM), (now FMI, Faculty of Mathematics and Informatics). In the period 1991-1996, she was a PhD student at the Department of Continuum Mechanics, FMI, SU. Later, in 2008, the candidate defended her PhD thesis on mathematical modelling of the fluid processes in packed-bed columns and received the doctorate, with a speciality in "Processes and Apparatuses for Chemical and Biochemical Technology" at IChE, BAS.

Assoc. prof. Petrova started her scientific career as a mathematician at the Institute of Mechanics and Biomechanics (now Institute of Mechanics), BAS in two short periods 1989–1990 and 1996. In 1996 she won the competition for a scientific researcher (nowadays equivalent to an assistant professor) at the IChE, BAS. Later, after receiving her PhD diploma in 2009, she continued as a chief assistant and from 2011 as an associate professor in the same institute. In total, the candidate has been working for more than 28 years in the IChE, BAS.

In the meantime, Assoc. Prof. Petrova has worked half-time by job-sharing at the European Polytechnical University, Pernik as an assistant professor and associate professor in Mechanics, consecutively since 2011.

The candidate participates in the governing body of the IChE as a chairperson of the scientific council of IChE from 2024 and as a chairperson of the colloquium of its scientists.

2. General characteristics of the scientific research and scientific applied activities of the candidate

The scientific and applied research activity of the candidate is mainly connected with the mathematical modelling for different types of engineering problems: flow distribution in packed-bed column apparatuses; composite materials degradation with application to wind rotor blade crack, delamination of energetic structures made by nanocomposites with or without the presence of graphene under the action of static or dynamic/electrical/thermal loads; optimal design of sustainable supply chains (SSC) in the dairy industry; and others.

The candidate is a leader of one national project financed by NSF, in the period 2021-2025 with the acronym КП-06-Н57/3/15.11.21, "Optimal safe load and geometry of layered nanocomposites at thermo-mechanical load". Moreover, she participated in 9 international scientific projects financed by DFG with the Technical University of Darmstadt, Germany in the period 2012-2022, as well as in 7 national projects. Four of them are financially supported by NSF. The treated problems of these projects are closely connected with the above-mentioned research topics.

3. Evaluation of the presented materials

Assoc. prof. Petrova presented 25 publications for participating in the competition: 23 - are papers in scientific journals and conference proceedings (all in English) and 2 - are book chapters in Bulgarian, by the national publishing house of BAS. The analysis of these publications shows that she is: a single author in 1 paper and the first author in 13 papers. All these works are published after 2011, i.e. after receiving the Assoc. Prof. Promotion.

The fulfilment information of the minimal national requirements for the promotion to Professor in the area "4.2. Chemical Sciences" is presented as follows:

1. Group B, 139 points (at minimum threshold 100 p.): habilitation work containing 9 papers, all in journals referred in Scopus; 3 papers - in journals Q2, 3 – in journals Q3, 2 – in journals Q4 and 1 – in journal with SJR.

2. Group Г.7, 241 points: 14 papers all in journals with ISI impact factor or impact rank SJR and quartiles: 1 paper in journal Q1, 6 – in journals Q2, 4 - in journals Q3, 3 – in journals Q4.

3. Group Г.8, 30 points for 2 book chapters in Bulgarian.

Group 7 – total 271 points (at minimum threshold 220 p.)

4. Group Д, 132 points (at minimum threshold 120 p.): 66 citations refereed in Scopus concerning 34 papers of the candidate.

5. Group E, 185 points (at minimum threshold 150 p.):

Group E.13 – PhD student with a defended thesis in co-supervision with Prof. Dzhonova – 50/2 = 25 points

Group E.14 – participation in 2 national projects, financed by NSF – 20 points

Group E.15 – participation in 6 international projects, financed by DFG, Germany – 120 points

Group E.16 – leader of 1 national project, financed by NSF – 20 points

Additionally, the candidate presented a full list of his publications in the period 1992 - 2024, which contains 43 papers in journals with ISI impact factor or impact rank SJR, 1 book chapter by international publishing houses and 2 – by national publishing houses, and 39 papers in peer-reviewed journals and conference proceedings.

6. Main scientific and scientific-applied contributions.

The problems, studied by the Assoc. Prof. Petrova, are in general from the domain of chemical engineering applications in energetics. A great part of the topics in the presented papers is developed in connection with the fulfilment of the candidate research project. She grouped her main scientific and applied research contributions in three thematic areas, as follows:

- *Research and evaluation of flow distribution in column apparatuses*
- *Modelling and optimization of composite and nanocomposite structures*
- *Designing optimal sustainable supply chains (SSC) in the dairy industry*

The habilitation work contains 9 papers concerning only the first thematic area, which are cited 28 times by independent authors. In one of the papers Assoc. Prof. Petrova is a single author. The other works are collective, where she is the first author in 6 of them and the second author in the remaining 2 papers. They occur as a prolongation of the previous research of the candidate, e.g., of her PhD thesis.

The irregular distribution of gas/liquid phases in packed-bed columns is one of the reasons for the difficulties during their functions. This could be caused by the design of the distribution devices or by the type of packing, the geometry of the columns, etc. These factors are studied and analysed by experimental and approximate methods. Based on the results of the habilitation work, Assoc. Prof. Petrova derived 7 significant contributions: 3 are connected with the gas distribution devices (GDD) considered in 4 papers and the remaining 4 contributions – with the liquid distribution systems in 5 papers.

The gas phase contributions comprise: (1.1) A new method for quantifying and locating the clusters (zones with equal velocities) has been developed. An idea to reduce the maldistribution by adding grids and gratings after the GDD is proposed; (1.2) New criterion equations for determining the hydraulic resistance of dry and wetted structured packing are derived; (1.3) The influence of the hydrodynamics of the gas flow on heat and mass transfer during flow around a single catalyst pellet - Raschig ring is studied numerically using two hypotheses of catalyst surface accessibility. The liquid phase contributions are the following: (1.4) Experimental set-up is designed of the uniform liquid sprayer and an added peripheral sprayer, by use of which the values of model parameters are obtained. This approach simplifies the measurement of flow velocity near the wall using a model formula from the dispersion model with data for different liquid distribution in Raschig Super-Ring (RSR) packings - RSR 0.7, RSR 1.5 and RSR 3; (1.5) A new procedure for identifying one of the model parameters, named "overlapping confidential intervals" solution, is developed and illustrated for RSR packing in the case when some of the coefficients of the dispersion model cannot be found by the method of minimum divergence between dispersion model and experiment. The obtained results predict good compatibility between the dispersion model and experimental data published by other authors; (1.6) Similarly to contribution

(1.5) (my opinion is both to be unified), some other methods for evaluation of the unknown parameters of the dispersion model are considered for large size columns. The model and experimental liquid distribution are in very good agreement; (1.7) The measuring of the liquid distribution in the packing layer includes a liquid collecting device (LCD) mounted under the packed bed. The proper design of the LCD is very important for obtaining correct information about the hydrodynamics in the column. The most popular construction of LCD is composed of a fixed number of concentric cylindrical sections, with equal or different cross-sectional surface areas. Several options for possible fragmentation of the number and width of individual sections in LCD are analysed and evaluated, based on simulations with a dispersion model and calculation of the maldistribution factor. It is shown also, that model parameter identification depends on the LCD fragmentation, especially in the wall zone of the packed column. A quantitative criterion for LCD design assessment is found, which includes the effect of fragmentation on the maldistribution factor to be less than a predefined value.

In the mathematical models of the upper commented papers, the candidate applied mainly statistical methods to derive the mentioned contributions. According to her classification of the contributions, the contributions (1.1), (1.2), (1.4) and (1.7) are marked as scientific-applied, while the rest (1.3), (1.5) and (1.6) – scientific. All contributions, except (1.3) are connected with the fulfillment of research projects.

The **second thematic area** covers 10 papers which are cited 15 times by independent authors. All the works are collective, where Assoc. Prof. Petrova is the first author in 4 of them and the second author in 3 papers.

The studied subject is extremely modern and has a direct connection with the production of new materials - composite and nanocomposite structures from polymers with graphene layers. It is supposed these materials have better mechanical, thermal and electrical properties than pure polymers. The application of such materials can be found in different industrial areas: blades of wind turbines, joints, sensors, building insulation materials, etc. The proposed works aim to model and optimise composite and nanocomposite structures subjected to static or dynamic mechanical, temperature and electrical loads at different rates of humidity.

The candidate classified the contributions of this area in the following way: (2.1) An analytical and simple 1D shear-lag model of the idealized straight line part of a wind rotor blade of the composite structures is proposed. The possible interface delamination under static mechanical, temperature, and electric loading and moisture change is analysed and detected. As a result, new analytical criteria for interface delamination are proposed, which predict the optimal choice of the upper loadings for safety work of wind rotor blade; (2.2) Applying the 1D shear-lag model, it is shown that at static load, the change in temperature and humidity strongly affect the value of the electrical gradient. There is a direct relationship between the voltage acting on the first piezoelectric layer of the composite structure and the delamination length, which makes it possible to predict the presence and extent of delamination by simply measuring the electric voltage; (2.3) At dynamic load of bi-material structures with different material properties the frequency interval could change significantly the solution character. The combined loads have important effects on the value of the interface shear stress and the

delamination length. A solution method based on shear lag and the Fourier method has been applied. The delamination could be avoided if stronger adhesives and thicker adherents are chosen. A new analytical equation for resonant frequencies is proposed, based on the obtained solutions since the resonance frequency depends on the densities, Young moduli, layers' width and adhesive shear stress; (2.4) For two of the studied composite structures - "lightweight joint" and "patch/layer", under static or dynamic loading, under the influence of an electric field and changes in the environment, a new multiparameter optimization procedure was developed. This optimization was performed by non-linear programming with genetic algorithms, which makes it possible to satisfy a criterion for a minimum or zero value of the delamination length at the interface of the structures. The optimal values of the geometry of the composite structures and those of the external influences were simultaneously determined; (2.5) A new two-dimensional stress-function method describing the stress transfer in a three-layered adhesive bonded graphene and polymethyl methacrylate (PMMA) nanocomposite structure, subjected to static and temperature load is proposed. Analytical two-dimensional stresses and strains in each of the layers of the nanocomposite structure were obtained by the variational principle of strain energy minimization. The comparison with literature experimental data and with literature results from the shear-lag model is good enough; (2.6) The temperature increase leads to an increase of the deformations in the nanocomposite layers, which are more visible in axial and normal deformations. The two-dimensional stress-function method is applied to model the axial strain distribution in a nanocomposite structure subjected to an axial tension load. The presented method is not appropriate for a few nanomaterial layers structure at an external strain near or above the elastic one, because of the appearance of a relaxation zone and the formation of wrinkles in the layers.

The contributions (2.1) - (2.4) are marked as scientific-applied and connected with the work of the candidate on the DFG projects during the last 10 years. The contributions (2.5) and (2.6) are scientific and refer to her leadership of the current research project with NSF, 2021-2025.

The mathematical models developed in papers 10 and 19 give the most important results, as shown by contributions (2.1) and (2.5). In my opinion, the works from this thematic group have the highest scientific contribution to the candidate's scientific production as a whole.

The **third thematic area** covers 4 papers which are cited 10 times by independent authors; all the works are collective.

The subject of this area concerns the design of optimal supply chains under different scenarios for production, dairy products, number of raw materials, different technologies, different numbers of suppliers, etc. and under different optimization criteria. The formulated and solved optimization tasks take into account various aspects of sustainability - environmental, economic and social under imposed restrictions.

The contributions of this thematic area according to the candidate are the following: (3.1) A deterministic optimization approach is proposed for the design of a product portfolio of a sustainable supply chain, including suppliers, plants and markets for the production of 2 types of dairy products, from 2 different raw materials and 2

types of technologies. The optimization is a search for maximum profit, taking into account environmental and economic aspects; the problems are formulated in terms of mixed-integer nonlinear programming and are solved under various imposed environmental pollution constraints; (3.2) The upper contribution is extended with added social impacts, applied to obtain the optimal design of a sustainable supply chains for dairy products, under 3 scenarios, each with a different optimization criterion: at maximum realization of supplied raw materials, at maximum profit, and maximum realization of products on the market. Only the third scenario leads to a satisfaction of the market's requirements; (3.3) The social impact assessment was included in the optimization problem and it has been shown its effect on the resulting optimal profit from dairy production. The best scenario for achieving the highest profit, lowest economic cost, and highest environmental cost is obtained by limiting both environmental and social cost results; (3.4) A new robust optimisation approach for handling the uncertainty of product demands in a dairy supply chains to produce different dairy products according to different recipes while satisfying environmental and economic criteria. Deterministic and robust optimization problems have been formulated and solved under nominal data for the product demands and three different uncertainty levels – 0.2, 0.5 and 1. The results show that the increase in the uncertainty level leads to decreased profit from the dairy supply chains with a relatively small standard deviation. The lowest average value of the supply chains' profit is obtained at the highest level of uncertainty. The total cost of the supply chains also does not change significantly with increasing levels of uncertainty. The largest cost value was obtained at the medium level of uncertainty.

In my opinion, the contributions (3.1), (3.2) and (3.3) could be unified. The results of the mathematical models of optimization are various and have a broad scope of application, which makes them quite useful. All contributions have a scientific-applied character and refer to the candidate's participation in the current research project with NSF, 2019-2024.

Additional publications to the first area, apart from the habilitation work:

Two book chapters are published in connection with the participation of the candidate in the research project with NSF 2016-2020. The presented results are part of the first thematic topic and the following two contributions are derived:

In Chapter 1, all performed experiments for measuring the radial distribution of the liquid phase (water) after a layer of disordered packings with an open structure in a pilot column with a diameter of 0.47 m. are described. The non-uniformity of the column-packed-bed inlet and outlet flows was also investigated and evaluated. Areas in the column with large-scale irregularity are identified.

Chapter 2 is dedicated to the theoretical study (mathematical modelling) of the radial distribution of the liquid phase after packing in an open structure using the dispersion model. The hypothesis of the influence of the fragmentation of the liquid collecting device (LCD) sections in the column wall area on identifying the dispersion model parameters was formulated and proved. Different variants of fragmentation of the LCD sections in the near-wall zone were simulated, and a quantitative criterion was chosen to determine the optimal variant. The verification of the dispersion model, the

methods for its parameter identification and the selection of the optimal LCD design have been successfully performed in second, third and fourth-generation packings for both pilot and industrial columns.

The first contribution has a scientific-applied character, while the second – one has with scientific character. Both chapters are connected with the participation of the candidate in the research project with NSF, 2016-2020.

7. Reflection of the candidate's results on the works of other authors

According to the presented citation list by the candidate, it is obvious that there are 165 citations of 37 papers. The papers presented to this competition have 53 citations up to now. The h-factor of Assoc. Prof. Petrova according to her citation list is 7. This is a good attestation of the significance of her work.

8. Critical notes and recommendations

I have no critical remarks concerning the presented papers. All of them are published in peer-reviewed journals, i.e., have passed the professional review process. I did not find any information about the candidate's participation in international/national conferences or any scientific events. The only mark of it is in the references of some papers.

9. The reviewer's impression of the applicant

I have known personally Assoc. Prof. Petrova for a long time. She was a student at the Department of Fluid Mechanics, BAS/SU, with which I collaborated at that time. I have a positive attitude toward her mathematical background, as well as for her profound knowledge of mechanics, which is evident from the brilliant research presented for this competition. The participation of the candidate in different international and national projects is a very good certificate for her capabilities. I recommend she extend these participations by applying to different international financing programs as a project leader. Also, I recommend she attract more graduate, post-graduate and/or PhD students in her research activities.

10. Conclusion

Following the scientific research activities of the candidate in total and having in mind the requirements for the academic position of "Professor" under the Law on Development of the Academic Staff of the Republic of Bulgaria and the Rules for its Implementation in BAS, **I find it reasonable to vote with full confidence in favour of the candidature of Associate Professor PhD Tatyana Stefanova Petrova for the academic position "Professor" of speciality "Processes and Apparatuses for Chemical and Biochemical Technology" in the professional area „4.2. Chemical Sciences" for the needs of the Institute of Chemical Engineering, BAS.**

5.01.2025 / Sofia

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