OPPONENT OPINION

Dissertation for acquiring of scientific and educational degree “Philosophy Doctor”

One candidate: Galina Stoyanova Lyutskanova-Zhekova

Topic of the dissertation: Numerical Modelling of Nonlinear Boundary Value Problems of Second and Fourth Order

Procedure Notifier: Department of Mathematical Modelling and Numerical Analysis, IMI, BAS, Sofia

Doctoral Program: Mathematical Modeling and Numerical Analysis

Opponent: Prof. Michail Todorov, PhD, Chair of Mathematical Modeling and Numerical Methods, Faculty of Applied Mathematics and Informatics by the Technical University of Sofia, Bulgaria, by order 445/07.10.2022 of the Director of IMI, BAS

Short biographical record of the applicant

Galina Lyutskanova was undergraduated Faculty of Mathematics and Informatics by the St. Kliment Ohridski University of Sofia, specialty “Applied Mathematics” in 2014. Two years later she graduated the specialty “Computational Mathematics and Mathematical Modelling”. In the period 2015-2017 she was part-time employed as a risk analyzer in Frontex International Services. Since 2017 she has been postgraduate student under program “Mathematical Modelling and Math Application” by the Institute of Mathematics and Informatics, BAS. In the same year Galina Lyutskanova is appointed as a part-time assistant in FMI, since 2020 – assistant in ordinary. Simultaneously she is a part-time mathematician in IMI, BAS.

The dissertation is written in English, volume of 160 pages, format B5+1/2, including 5 chapters and 1 appendix, 27 figures, 1 table and bibliography of 142 items.

1. General characterization of the dissertation problem

To construct of adequate rheological models requires simple mathematical models in order to adapt to experimental data and to get a reliable information about the rheological parameters (viscosity, slipping, threshold tension, etc.). Such kind of activities require the same recognition of both the real processes and the corresponding mathematical tools for analytical, computational and software implementation of the models and treatments. The subject possesses an explicit ground and needs practical applications the latter being a successful motivation to conduct them. All that presumes the necessary mathematical qualification and skills, that the applicant undoubtedly has and cleverly executes.

2. Current state of the problem

The classical and new fluid materials have varied applications in chemical, food, wine and tobacco industries as well in the pharmaceutical technologies. These activities require profound study and prediction of their rheological properties related to the skin and eye effect, stability, decomposition, etc. Briefly speaking a mathematical description of the materials is needed. The character of the applied problems in question (foams, emulsions, solders, cells, tissues, liquids, etc.) requires mathematical models of non-Newtonian fluids, where the surface tension over their material boundaries are not constant. They are called complex.

3. Methods of investigation

There are two approaches to study and investigate the problems in the thesis – the molecular dynamics and hydrodynamics. Having in mind the specifics of the problems under consideration the applicant directed to the second one where she supposed the fluid is continuous and more adequate for 3D problems. Within the frame of continuum mechanics the complex fluid is modelled by the balance laws of mass, momentum, and energy. These models, however, are not closed. In order to close them are used various semi-empirical hypotheses about the relation between the tension tensors and the deformation. Generally speaking the latter leads to nonlinear systems of order four. The problem consists in a deformation of material boundaries, their complex shape and rheological behavior though the volume phases are incompressible. The methods are based on the Laplace equation with bi-operator of order four and Stokes' equation, which is reduced to a nonlinear system of 4 ODEs. The difficulties to treat and solve them are indispensable. All that requires a flexible approach to solve numerically the respective boundary-value problems. In my opinion, Mrs. Lyutskanova puts it into practice professionally. It is related to the methods and software as well as to the quality and significance of the obtained results.

4. Review and evaluation of the scientific achievements

The PhD thesis considers three applications of boundary-value problems in the physics-chemistry and the biology as follows

- Computing of potentials' distribution in two fluid phases (polar and non-polar) and in spherical colloid dielectric particle attached to a plane boundary between them;
- Determination of the drag of a spherical colloid particle attached to a plane boundary between two incompressible viscous fluids, which is moving parallel with a constant velocity;
- Study the effect of boundary rheology (tangential mobility and immobility) over the dynamics of long bubble in a short cylindrical tube, caused by the flow simultaneously operated by a gravity and pressure.

Chapter 1 actually is an introduction to the thesis. The next 3 chapters are the real contribution. Three applications of boundary-value problems considered lead to linear or strongly nonlinear models of order two or higher.

The interface between large proteins and colloid particles attached to the boundary between two fluids is considered in Chapter 2. It is supposed to be due to van der Waals' electrostatic and capillary forces, while the gravity is neglected. The deformation is a result of the electrostatic pressure distribution over them and the related to it electro-flooding force. The problem in question includes empirical and theoretical parts. The latter is based on the balance condition of the charge, from where the surface deformation is determined.

The second problem consists in two complex subproblems and they are studies in Chapter 3. The first one is a modelling of the range of big number molecules and colloid particles on the surface as well as the resulting drags acting them due to the Brown motion caused by the van der Waals, electrostatic and capillary interactions.

The necessity to pose and solve the second problem evolves from the lack of a direct microscopic measure method for the three-phase contact angle. By a measure of the tangential velocities of particles one determines the drag. The latter needs a fast and precise numerical method to compute the drag for a given three-phase contact angle, aiming to run empirically the value of the angle.

One of the hard problems in the modelling of physics-chemistry processes is to get the shape of the material boundaries both in static and dynamical modes having in mind their hydrodynamical stability. To illustrate that in Chapter 4 is considered the motion of a long bubble in a cylindrical capillary under the influence of the pressure gradient (Poiseuille flow) and/or the gravity. The bubble surface is allowed to be free, i.e., a tangentially moving surface in the classical frame; tangentially fixed but deformable. For instance, biological membranes, surfaces with adsorbed with active substances, etc. The problem can be a part of more complicate computations like drops and bubbles motion in a rocky porous media or a motion of biological liquids in the human veins. Few exact solutions for motion under the gravity and the pressure are known. They concern very small velocities (the Bretherton problem) as well as a bubble with a free surface under pressure gradient. The complexity is caused by the necessity of considerable computational resources and implementations, which do hard even impossible to compute complex fluids and material boundaries.

The actuality of the problems under the consideration in the PhD thesis, the novelty in the methods of their solution both from physical, chemical and mathematical point of view, comparison with the known so far publications, and the basic strategies are described in Chapter 5. The main contributions are resumed in 3 points. Chapter 5 actually plays the role of Author Contributions. They are as follows

1. The mathematical model about the distribution of electrostatic potentials in dielectric media (two fluid phases and a spherical colloid particle attached to a plane boundary between them) contains 3D Laplace equations, continuous functions and Neumann boundary conditions. The problem is solved numerically by developed for this purpose efficient and fast algorithm. The numerical implementation requires a prior toroidal coordinate system rendering the original boundaries in coordinate lines; analytical investigation of the weak singularity on the three-phase contact line; an implementation of a self-consistent order two, that uses ADI method. It is supposed the water permittivity is a finite having in mind all the dielectric media.

2. The translation motion of a spherical colloid particle attached on the plane boundary between two viscous incompressible fluids is described by the Stokes equations for the velocity field and the pressure in 3D regions. It is supposed the velocity field and tangential surface tensions between both fluids are continuous while the velocity vector on the particle surface is given. The problem is re-formulated in the terms of vector and scalar potentials of the velocity

and the pressure. The original 3D BVP is rendered to 2D one with respect to the first Fourier modes related to the polar angle. This approach permitted to accelerate the numerical realization many times compared to a previously used method. The rest part of Contribution 2 repeats the algorithms and technics from 1 and will be skipped in the review.

3. Motion of a long bubble with free boundary (the classical case) or tangentially motionless boundary (biological membrane, surface with attached active substances, etc.) through a cylindrical capillary under gravity and pressure. The approach to such kind of problems is semi-analytical. The model consists in 3D Stokes' equations for given velocity profile far from the bubble, sticking condition on the capillary wall, tangential and normal projections of the dynamic boundary conditions over the deformable surface of the bubble. In order to get approximations for the bubble smooth shape of zeroth and first order the analytic Stokes solution for small slopes of the surface tangent is used. Next, the obtained solutions are substituted for the normal projection of the dynamical boundary condition. From there a system of four nonlinear ODE of order one follows for the arc length with one unknown parameter (the capillary pressure on the bubble point). Further, the BVP of order four with respect to the shape by running the above parameter is solved numerically up to getting a closed profile. As a result the above described method confirms very well the known experimental data, increases more than 100 times the application region of the earlier known analytical methods. Also, it explains the complex dynamics of long bubbles under the simultaneous influences of gravity and pressure concerning classical and tangentially fixed surfaces.

5. Opinion of the author contributions

The author information correctly tells on the achievements and accents of the dissertation thesis. The achievements are scientific and scientific with practical direction. The analyses and criteria can be used direct in colloid physics-chemistry, oil production, biochemistry. In my opinion, the achievements are joint and the applicant takes leading role. All of them belong to the directions "Adding to existing knowledge" and "Applications in practice". The investigation of such kind of problems needs a mutual relation between the theory and experiment – mutual complement and adding to knowledge.

6. Critical remarks and recommendations. Literary knowledge

My impression from the dissertation thesis is positive. Written in English, the statement is concise and clear. I have not any remarks and criticisms. The literary knowledge is based on contemporary sources.

7. Publications

The results are presented and verified on few conferences and seminars in BG and abroad. They are published in *Lecture Notes in Computer Science, Progress in Industrial Mathematics (Springer), Physics of Fluids*. All of them are co-authored. *Physics of Fluids* possesses IF 4.98 (2021), belongs to the quartile *Q1* and already generated 2 cites. The publication in *Lecture Notes in Computer Science* has SJR and one more cite.

More details one can find in the table below

Papers – 3 numbers	Abroad - 3 numbers *Physics of Fluids, LNCS, Progress in Industrial Mathematics*
Conference reports and presentations – 7	In BG*: seminar in section Math Modelling and Numerical analysis, IMI-BAS, Spring Session of FMI, BIOMATH 2018, NM&A 2018* Abroad: *20th European Conference on Industrial Mathematics, Budapest, , Mathematics in Applications-Novosibirsk 2019, International Virtual Conference on Mathematical Science-2021*

8. Importance and contribution to the practice

The results obtained in the dissertation thesis contribute to the computational physics-chemistry of colloid particles in two-phase media. Let us emphasize that the results are model allowing direct confirmation and prediction in the experiment. They can be applied successfully the latter being a precondition to new meaningful problems

9. Opinion of the abstract of the dissertation

The abstract corresponds to the matter of the dissertation completely.

10. Personal impression

I do not know personally Galina Lyutskanova.

Conclusion

Gaining an impression for the doctoral thesis (dissertation) of the applicant and having in mind the legal rules and criteria (LDASRB, its regulations in BAS and specific requirements in IMI) I **rate positively** the dissertation. On the strength of virtue of the law **I propose Galina Stoyanova Lyutskanova-Zhekova** for scientific and educational degree Philosophy Doctor (PhD) in Field of Higher Education: 4. Natural Sciences, Mathematics and Informatics, Professional Direction 4.5 Mathematics, Doctoral Program: Mathematical Modeling and Numerical Analysis.

Opponent

Prof. Michail Todorov

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Sofia, December 10th 2022