ABSTRACT

for the degree Dissertation on the topic “Mathematical justification of numerical methods for solving atmospheric boundary layer equations” for the degree Doctor of Philosophy (PhD) in the educational program “8D05405 – Computational Sciences and Statistics”
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Relevance of the research topic. This dissertation proposes a modified implicit three-step MAC scheme for the Navier–Stokes equations with a correct approximation of pressure boundary conditions; it increases the stability and accuracy of the numerical method, and its validity is rigorously justified for atmospheric applications.

The purpose and objectives of the study. The purpose of the dissertation is to develop effective difference schemes for the numerical solution of the Navier-Stokes equations and the atmospheric boundary layer model, and to analyze their approximation properties, stability, and convergence. Conducting numerical experiments using the developed scheme.

The following research objectives were set:

1. Formulation of the Navier-Stokes problem and problems for numerical solution of atmospheric boundary layer equations and their approximation;
2. Development of an algorithm for a modified three-stage splitting scheme by physical processes for the numerical solution of the Navier-Stokes problem;
3. Approximation of the Neumann boundary conditions for the numerical solution of the elliptic pressure equation;
4. Investigation of stability and convergence issues of the developed modified three-stage splitting scheme for Navier-Stokes equations;
5. Application of the developed modified three-stage splitting scheme by physical processes for numerical solution of the atmospheric boundary layer problem;
6. Investigation of issues of stability and convergence of the developed modified three-stage splitting scheme for atmospheric boundary layer equations;
7. Conducting numerical experiments and developing the program code;
8. Application of the program code to create a map of the information and analytical platform.

Research methods. The dissertation uses the finite difference method, the marker and cell method, the splitting method by physical processes, the a priori estimation method to substantiate the stability and convergence of the solution of a difference problem to an exact solution of a differential equation, the integro-interpolation method to obtain a priori estimates, the run-through method for numerical implementation of the algorithm, the high-level Python programming language and its modules and libraries for writing software code and modeling.

The scientific novelty of the work. An algorithm of a modified three–stage splitting scheme for physical processes with implicit difference schemes for numerical solution of Navier-Stokes equations has been developed and implemented. Unlike classical schemes, the new technique makes it possible to obtain a priori estimates of the second derivative of the velocity vector and the pressure gradient for the Navier-Stokes equations and the atmospheric boundary layer equations, and also performs calculations in large time steps.

An essential element of the novelty is the study of the approximation properties of the boundary conditions for pressure, which made it possible to increase the accuracy of the numerical solution and ensure the correctness of the application of the developed scheme.

The issues of approximation, stability, and convergence of the proposed scheme for the Navier–Stokes equations are theoretically investigated, which provided a rigorous mathematical validity of the developed method. In addition, a computational analysis of the effectiveness of the new scheme was performed, during which its advantages over known approaches were evaluated, including in terms of accuracy, convergence rate, and the amount of estimated time. Numerical calculations confirm the theoretically obtained results on the correctness of the difference scheme.

The developed algorithm was applied for the first time to the numerical solution of the atmospheric boundary layer model, which made it possible to adapt the splitting scheme to the tasks of environmental modeling. Studies of the stability and convergence of the scheme in relation to the equations of the atmospheric boundary layer have also been conducted, which expands the scope of the method and confirms its universality.

Scientific statements submitted for protection:

1. An algorithm has been developed for a modified three-stage splitting scheme by physical processes for the numerical solution of the Navier-Stokes equations;
2. The approximation properties of boundary conditions for the numerical solution of the elliptic pressure equation are studied.;
3. The issues of stability and convergence of the developed modified three-stage splitting scheme for the Navier-Stokes equations are investigated and proved.;
4. A computational analysis of the efficiency of the developed modified splitting scheme in comparison with classical schemes was performed, which made it possible to identify its advantages in terms of accuracy and stability of the numerical solution.;
5. The developed modified three-stage splitting scheme by physical processes is applied to the numerical solution of the atmospheric boundary layer problem.;
6. The stability and convergence of the developed modified three-stage splitting scheme for atmospheric boundary layer equations are investigated and proved.;
7. Numerical experiments have been carried out and a program code has been developed;
8. The program code is used to create a map of the distribution of pollutants in the urban atmosphere in an information and analytical platform.

Theoretical and practical significance of the research. From a theoretical point of view, effective numerical methods for solving atmospheric boundary layer equations and Navier-Stokes equations have been developed and substantiated, including a three-stage splitting scheme and methods for clarifying pollutant emissions. The issues of approximation, stability, and convergence of the proposed numerical algorithms are investigated.

The practical significance lies in the development and implementation of a numerical algorithm for modeling the spread of impurities in the atmosphere of industrial cities, tested on the example of Ust-Kamenogorsk. A Python software package has been developed, integrated into an information and analytical platform to support decisions in the field of environmental policy.

Approbation of the work. The main research results were presented at the following conferences:

- 6th International Conference of Mathematical Sciences (ICMS 2022), 20 – 24 July 2022, Maltepe University, Istanbul, Turkey;
- Sixth International Conference on Analysis and Applied Mathematics (ICAAM 2022), from October 31 to November 6, 2022, Antalya, Turkey.
- Computational and Information Technologies in Science, Engineering and Education (CITech-2022), October 12-15, 2022, Almaty, Kazakhstan.
- VII World Congress of Mathematicians of the Turkic World (TWMS Congress-2023), September 20-23, 2023, Turkestan, Kazakhstan.
- Inverse and incorrect problems in Natural Science and artificial Intelligence, April 16-20, 2024, Almaty, Kazakhstan.
- Weekly seminar “Analysis and Applied Mathematics" organized by Bahçeşehir University, Istanbul, Turkey, Analysis & PDE Center, Ghent University, Ghent, Belgium, Institute of Mathematics & Math. Modeling, Almaty, Kazakhstan. June 13, 2023, Istanbul, Turkey.
- Seminar "Modern problems of applied and computational mathematics", January 5, 2025, Almaty, Kazakhstan.

Publications. The following papers were published based on the materials of the dissertation:

1. Temirbekov, N., Malgazhdarov, Y., Tamabay, D., Temirbekov, A. Mathematical and computer modeling of atmospheric air pollutants transformation with input data refinement. Indonesian Journal of Electrical Engineering and Computer Science.-2023. Vol.32, No.3.-P. 1405-1416. (DOI: 10.11591/ijeecs.v32.i3.pp1405-1416, (Scopus percentile– 61, SJR= 0.272, Scopus quartile – Q3)
2. Temirbekov, N., Malgazhdarov, Y., Tamabay, D., Temirbekov, A. Atmospheric modelling of photochemical transformations of pollutants: Impact of weather conditions and diurnal cycle (Case study: Ust-Kamenogorsk, Kazakhstan). Mathematical Modelling of Engineering Problems, –2023. Vol. 10, No. 5. – P. 1699-1705. (https://doi.org/10.18280/mmep.100520, Scopus percentile– 47, quartile – Q3)
3. Temirbekov, N. Tamabay, D., Tanashova, M. Spread of harmful substances in the atmosphere of industrial cities of Kazakhstan: modeling and data refinement. Indonesian Journal of Electrical Engineering and Computer Science. —2025, Vol.

37(1), pp.636-647; https://doi.org/ 10.11591/ijeecs.v37.i1.pp636-647. (Scopus percentile – 55, quartile – Q2)

4. Temirbekov, N., Temirbekov, A., Kasenov, S., Tamabay, D. Numerical Modeling for Enhanced Pollutant Transport Prediction in Industrial Atmospheric Air. International Journal of Design and Nature and Ecodynamics. —2024, Vol. 19(3), pp. 917–926; https://doi.org/10.18280/ijdne.190321. (Scopus percentile – 54, quartile – Q2)

Articles included in the list recommended by the of the Ministry of Foreign Affairs of the Republic of Kazakhstan have been published:

Tamabay, D. and Zhumagulov, B. Stability of the three-step splitting scheme for the Navier-Stokes equations in the context of the large particle method. Bulletin of KazNPU named after Abai, Series "Physical and Mathematical Sciences", 2024, 85, 1 (Mar. 2024), 51-62. DOI:https://doi.org/10.51889/2959-5894.2024.85.1.005

Monograph published:

Temirbekov N.M., Madiyarov M.N., Tukenova Z.A., Malgazharov E.A., Kasenov S.E., Baigereev D.R., Temirbekov A.N., Tamabay D.O., Temirbekova M.N., Abdoldina F.N., Dedova T.V., Nasyrova M.S. Unified ecosystem for monitoring data collection and processing atmospheric air of industrial cities: a monograph / Under the general editorship of N.M. Temirbekov; coll. author. Almaty: Everest, 2024 - 330 pages.

A chapter of the monograph has been published:

Tamabay, D., Zhumagulov, B., Temirbekov, A. Mathematical Issues of Difference Schemes for Atmospheric Boundary Layer Equations. Trends in Mathematics. —2024, Vol. 6, pp. 185–196. Springer. https://doi.org/10.1007/978–3–031–62668–5_18.

Utility model patents have been obtained:

1. "Method of remote monitoring of atmospheric air" (application number No. 2024/0192.2) No. 9055, dated February 12, 2024, issued by the RSE "National Institute of Intellectual Property" of the Ministry of Justice of the Republic of Kazakhstan.

2. "Device for remote monitoring of atmospheric air" (application number No. 2023/0409.2) No. 8629, dated October 27, 2023, issued by the RSE "National Institute of Intellectual Property" of the Ministry of Justice of the Republic of Kazakhstan.

Copyright certificates have been obtained:

1. "Geoinformation system for monitoring the atmospheric air of industrial facilities, taking into account photochemical transformations based on digital technologies" No. 32823 dated February 20, 2023, issued by the RSE "National Institute of Intellectual Property" of the Ministry of Justice of the Republic of Kazakhstan.

2. "Development of a program based on machine learning methods to assess the negative impact of air pollution on health No. 42532 dated January 31, 2024, issued by the RSE "National Institute of Intellectual Property" of the Ministry of Justice of the Republic of Kazakhstan.

The structure and scope of the dissertation. The dissertation is presented in handwritten format in Russian and includes a title page, a table of contents, an introduction, three main sections, a conclusion and a list of references from a number of sources. The total volume of the work is 124 pages containing 9 illustrations, 1 table, 200 literature sources and 4 appendices.

The main content of the dissertation:

The dissertation is devoted to numerical modeling of viscous incompressible hydrodynamics and pollutant transport in the urban atmosphere, with an emphasis on stable and convergent finite-difference schemes for the Navier–Stokes equations and their applied implementations.

Chapter 1 examines the lid-driven cavity problem. A finite-difference approximation is proposed featuring a modified three-stage splitting by physical processes, which enables computations with large time steps. Boundary conditions (including for pressure) are correctly approximated. Stability and convergence of the scheme are proved.

Chapter 2 develops a model of the atmospheric boundary layer over an industrial city, taking into account turbulence, a heterogeneous underlying surface, and localized sources; a difference scheme is constructed and its stability and convergence are justified. The model is intended for environmental forecasting and air-quality control.

Chapter 3 presents numerical experiments: flow visualization, a comparison with the classical two-stage splitting scheme (demonstrating the advantage of the proposed approach), and simulations of pollutant dispersion.

In conclusion, an information-analytic system for air-quality monitoring in cities of Kazakhstan is developed, integrating modeling with analysis and visualization.