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"8D05405 Computational Sciences and Statistics"
for the educational program
for the degree of Doctor of Philosophy (PhD)
dissertation on the topic "Solution of computational hydrodynamics in areas with complex geometry using adaptive networks"

Abstract

The Navier–Stokes equations, describing the motion of a viscous incompressible fluid, represent a fundamental model in modern hydrodynamics and are widely applied in the numerical modeling of flows within complex engineering systems. The curvilinear coordinate method was employed to solve the Navier–Stokes equations in complex geometric domains where coefficients exhibit rapid variations.

The proposed numerical method was verified by solving the Roache test problem. In the problem under consideration, the weak solution obtained via FEM was compared with the approximate solution derived from the FDM, demonstrating a high degree of agreement between the two. A weak solution to the boundary value problem for the Navier–Stokes equations in cylindrical coordinates was determined, with its stability and convergence rigorously proven.

Program code was developed on the FEniCS computing platform for the numerical simulation of the boundary value problem for the weak solution of the Navier–Stokes equations in terms of variables u, v, p The axial and radial velocities were determined for a pipe with a variable radius. The velocity vorticity ω was expressed in a "special" manner to determine the stream function ψ. A program was developed in Python 3.11 for the numerical simulation of the Navier–Stokes equations in terms of ψ, ω variables within arbitrary curvilinear coordinates. A stepwise integration method was proposed for the numerical computation of pressure.

Research objective. Numerical modeling of viscous incompressible fluid flow in complex geometric domains using adaptive grid methods, alongside a theoretical and numerical validation of the stability, accuracy, and computational efficiency of the proposed methodology.

Object of study. Numerical analysis of Navier–Stokes equations in complex geometries. This study focuses on the generation of adaptive curvilinear grids and the application of the finite element method (FEM). The Navier–Stokes equations are transformed into arbitrary orthogonal curvilinear coordinates to derive a stable numerical scheme. Conducting simulations for various Reynolds numbers to investigate accuracy and computational efficiency. Verifying the developed method using test cases and performing an analysis of numerical results obtained via the finite element method (FEM) and the finite difference method (FDM).

Research methods. In this work, numerical and computational modeling methods based on the Navier–Stokes equations for viscous incompressible fluids are employed. To solve the system of equations, the method of transformation to arbitrary orthogonal curvilinear coordinates, the finite difference method, and the finite element method are utilized.

Furthermore, structured and unstructured grids are considered for the discretization of the computational domain, and boundary and initial conditions are appropriately assigned. The stability and convergence of the calculations are analyzed, and a comparative analysis is performed to evaluate the accuracy of the obtained results. Numerical simulations are implemented via modern computational software, with modeling results presented through comprehensive graphs and tables.

Scientific novelty. Main results submitted for defense.

1. A curvilinear coordinate method was developed to solve Navier–Stokes equations with complex geometry and rapidly varying coefficients.

2. Verification of the proposed numerical solution method through the resolution of the Roache test problem.

3. The weak solution of the considered problem obtained via FEM and the approximate solution obtained via FDM were compared, demonstrating that they coincide with high precision.

The weak solution to the boundary value problem for the Navier–Stokes equations in cylindrical coordinates was determined, and its stability and convergence were proven.

5. A program code was developed on the FEniCS computing platform for the numerical computation of the boundary value problem for the weak solution of the Navier–Stokes equations in terms of u, v, p variables. The axial and radial velocity for a pipe with variable radius was determined. To find the stream function, the velocity curl was expressed in a "special" form.

6. A program was developed in Python 3.11 to numerically solve the Navier–Stokes equations in arbitrary curvilinear coordinates using ψ, ω variables, for which a copyright certificate has been obtained. A stepwise integration method is proposed for the numerical calculation of pressure values.

Approbation. Presented and discussed findings at 7 scientific seminars regarding the dissertation work.

1. Темирбеков Н.М., Керімақын А. Solving differential equations in two-dimensional space using the method of creating an adaptive grid. // Proceedings of the VII World Congress of Turkic World Mathematicians (TWMS-2023). – Turkestan, Kazakhstan, 20–23 September 2023. – Turkic World Mathematical Society, 2023.

2. Nurlan Temirbekov, Kerimakyn Ainur, Studies of the dynamics of catalytic converters of automobiles using the NavierStokes equations in arbitrary curved coordinates, "Computational and Information Technologies in Science, Engineering and Education" (CITech-2024) and made a presentation entitled,Almaty, October 23-24, 2024.

3. Temirbekov N.M., Kerimakyn A., Mathematical and computer modeling of a catalytic converter using Navier-Stokes equations in curvilinear coordinates, Mathematical modeling, equations of mathematical physics and geometry, 60th Anniversary of the Institute of Mathematics and Mathematical Modeling, april_conference_2025.

4. Kerimakyn Ainur, Mathematical and Computational Modeling of Catalytic Converter Using Navier–Stokes Equations in Curvilinear Coordinates,ISAAC CONGRESS ASTANA 2025,in the 15nISAAC congress ,held at Nazarbayev University,Kazakstan, from July 21 to July 25,2025.

5. Nurlan Temirbekov, Kerimakyn Ainur., Mathematical and Computational Modeling of Catalytic Converter Using Navier–Stokes Equations in Curvilinear Coordinates, ABSTRACT BOOK of the X International Scientific Conference on "MATHEMATICS, MECHANICS AND INFORMATION TECHNOLOGIES", al-Farabi Kazakh National University, Republic of Kazakhstan, Almaty, September 24–26, 2025.

6. Kerimakyn A., Aytuganova Zh., Ibragimova D., Mathematical modeling of adaptive mesh generation based on the equivalent distribution method in complex geometric domains, – Almaty: "Informatics and Applied Mathematics".

7. N. M. Temirbekov, A. Kerimaqyn, Application of curvilinear coordinate methods for flow modeling in complex geometries, Kazakhstan in the era of artificial intelligence: problems and prospects for the development of the agro-industrial complex and engineering, Almaty, April 16-17, 2026.

Publications. Four works have been published based on the results of the dissertation research, including:

— 2 articles in the international Scopus database

1. Nurlan Temirbekov, Kerimakyn Ainur, Mathematical and Computational Modeling of Catalytic Converter Using Navier–Stokes Equations in Curvilinear Coordinates,Mathematics 2025, 13(8),1355; https://doi.org/10.3390/math13081355

2. Temirbekov N., Khakimzyanov G., Kerimakyn A. Application of the Curvilinear Coordinate Method for the Numerical Solution of the Navier–Stokes Equations in Domains with Complex Boundaries // Computation. – 2026. – Vol. 14. – No. 3. – Article 58. – DOI: 10.3390/computation14030058

3. Temirbekov, Nurlan M., & Kerimakyn, Ainur. Methods for Creating Orthogonal Curvilinear Grids in Media with Complex Geometry. Bulletin of the National Engineering Academy of the Republic of Kazakhstan, 2025, 3(97), 242–250.

4. Kerimakyn A., Shekerbaeva Sh. , Kerimakyn C. , Talpakova B. Construction of an Adaptive Grid in a Domain with Complex Geometry Based on the Equivalent Distribution Method. Bulletin of Abai Kazakh National Pedagogical University. Series of Physical and Mathematical Sciences, 2025, 2(90), 72–80. https://doi.org/10.51889/2959-5894.2025.90.2.006.

Structure of the dissertation. The dissertation shall comprise normative references, an introduction, three main chapters (divided into sub-sections), a conclusion, and a bibliography.

The introduction must provide an overview of the research relevance, research objectives, mathematical modeling of the problems investigated, findings

submitted for defense, the object of study, the scientific novelty and theoretical-practical significance of the results, as well as details concerning the academic approval process, the author's publications, and the scope of the dissertation.

The **first section** of the dissertation considers the weak formulation of an initial-boundary value problem in cylindrical coordinates for the Navier–Stokes–Brinkman equations, which describe the flow of a viscous incompressible fluid in a porous medium. The problem is formulated in a variational form for the axisymmetrical case, and the weak solution is defined in Sobolev spaces; A priori estimates ensuring the stability of the solution were derived based on the energy method. Numerical simulations were carried out using the FEniCS platform. As the Reynolds number increases, the maximum value of the stream function ψ_{max} increases, a phenomenon attributed to the intensification of inertial effects and the expansion of the recirculation zone.

Furthermore, an analysis was conducted across various grid densities. The results demonstrate that the difference between solutions obtained with grid densities of 350 and 450 is negligible, thereby confirming that grid independence has been achieved and verifying the stability of the applied finite element method model.

In the **second chapter** of the dissertation, the Navier-Stokes equations are transformed from a cylindrical coordinate system to a general curvilinear coordinate system, and a finite difference scheme is constructed for the resulting equations. Employing the orthogonal curvilinear grid method, the numerical solution of the equations is obtained based on these grids. To solve the system of equations, a three-level finite difference scheme was employed, and an iterative method was proposed.

The developed algorithm ensures grid orthogonality and the numerical stability of the solution. Calculations performed within the Reynolds number range of Re = 10–1000 demonstrate strong agreement between the obtained results and the benchmark data reported by Roach, as well as the research conducted by Napolitano M. and Orlandi P.

In the **third section** of the dissertation, the system of Navier–Stokes equations used for modeling the catalytic converter is based on physical laws. The transition from cylindrical coordinates to arbitrary curvilinear orthogonal coordinates was justified through rigorous mathematical expressions. Established methods were utilized to generate orthogonal grids for curvilinear domains.

The finite difference method was employed to solve the equations, and the computational process was executed based on a three-level algorithm. The stability and convergence of this scheme have been theoretically proven. The numerical solution was obtained using the Python 3.11 programming language within a Jupyter environment.

Degree of implementation. The results presented in this dissertation focus on advancing numerical methods for approximating the Navier–Stokes equations, improving their stability and convergence, and enhancing computational accuracy for complex geometric domains. Furthermore, the proposed approaches allow for the efficient use of computational grids and enhance the reliability of numerical algorithms.

The practical significance of this research is defined by the applicability of

the developed method to model fluid flows in automotive catalytic converters and other engineering systems characterized by complex geometries.

Field of Application. The model presented in this dissertation can be enhanced by incorporating thermodynamic and chemical reaction effects, which are essential for evaluating the overall efficiency of the catalytic converter. The model developed in this dissertation can be applied to determine the geometry of the catalytic converter and to simulate the processes occurring within it. This model can be applied not only in the automotive industry but also in the fields of industrial gas purification, gas reactors in chemical production, and environmental protection systems.

The candidate's contribution to the research article. The research findings derived from the doctoral dissertation have been disseminated through two publications in journals indexed in the Scopus database and two articles in domestic peer-reviewed journals. The candidate demonstrated a comprehensive grasp and critical synthesis of the methodologies and theoretical frameworks applied throughout the research articles. Furthermore, the results obtained in each section are directly attributable to the candidate. However, in instances requiring specific theoretical conceptualization, the candidate consulted with both domestic and international supervisors.