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Calculation of impurity propagation in laminar flow of incompressible fluid inside a diffuser and comparison of performance of some calculation schemes

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Abstract

This study develops and tests a new finite-difference scheme named the TIIAME NRU scheme. It focuses on modeling impurity transport in laminar flows of incompressible fluids within diffusers. This approach addresses the conservativity loss issues seen in older numerical methods. The methodology focused on creating the TIIAME NRU scheme. This was done by strictly following the laws of mass and momentum conservation. It was compared to the classical Courant-Isaacson-Rees scheme. This was done through numerical tests on problems with known solutions in two-dimensional diffusers. Four cases were analyzed: incompressible flow in an expanding diffuser; compressible medium flow; variable cross-section flow; axisymmetric problems in cylindrical coordinates. The findings indicate that the proposed TIIAME NRU scheme demonstrates superior performance in maintaining conservativity, particularly in complex geometries with velocity sign changes. The new scheme remains stable with 15-20% larger time steps without accuracy loss, maintains strict conservation laws even under compressible flow conditions, and shows invariance to coordinate system choice. Numerical experiments confirmed that the classical scheme loses conservativity when impurity flows collide or merge, while the TIIAME NRU scheme preserves mass conservation. In conclusion, the TIIAME NRU scheme provides a robust solution for impurity transport calculations in complex geometries, offering improved stability and conservativity over traditional methods, and can be extended to three-dimensional problems with minimal algorithmic modifications. The practical implications of this research are significant for applications in jet engine design, gas burner optimization, and power plant calculations, where accurate impurity transport modeling is critical, and its improved computational efficiency and stability make it suitable for integration into industrial CFD packages.

Keywords: Computational fluid dynamics (CFD), Conservative finite-difference scheme, Diffuser, Impurity transport, Laminar flow.

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1. Introduction

1.1. Background

Computational fluid dynamics (CFD) is a critical component of modern engineering. It is used in a variety of processes, including power plant optimization and jet engine design. CFD problems are often solved using finite-difference schemes to solve the fundamental equations of fluid motion, including those related to momentum and mass transfer. The safety of industrial systems and the quality of engineering solutions depend on the accuracy and reliability of these numerical methods.

Equations used in hydrodynamic and aerodynamic problems include calculations of mass and momentum displacement in space. For solutions derived from these equations to be practically useful, they must meet several important requirements: stability, transportability, conservativity, adequacy, and invariance. If even one of these characteristics is violated, the numerical solution may be unsuitable for real engineering calculations.

1.2. Problem Statement

Existing finite-difference schemes, particularly the widely used Courant-Isaacson-Rees (CIR) scheme, have significant limitations when applied to flows with complex configurations. Often, these schemes are not conservative when dealing with velocity fields that change sign in space or time. Such conditions are frequently encountered in calculations involving diffusers and confusers. These limitations are especially noticeable in two- and three-dimensional problems, where variable velocity fields are common.

The loss of conservativity in numerical schemes is a fundamental problem in computational fluid dynamics. Violating the laws of conservation of mass and momentum leads to inaccurate solutions and erroneous predictions in important engineering areas such as turbomachinery, combustion chambers, and heat exchangers.

1.3. Research Gap

Despite extensive research in computational fluid dynamics, a significant gap remains in developing computational schemes that possess the following key properties: stability, transportability, conservativity, adequacy, and invariance. Most existing schemes fulfill some of these properties but are inferior in others. For instance, the Courant-Isaacson-Rees scheme offers good stability and transportability. However, it exhibits significant conservativity loss in complex velocity fields.

Additionally, incorporating new computational schemes into existing CFD tools often requires substantial algorithmic modifications, hindering practical applications. Therefore, there is a need for conservative schemes that can easily integrate with existing computational environments. These schemes should also provide high accuracy and stability under different flow conditions.

1.4. Objectives

This research aims to develop and validate a new finite difference scheme for modeling impurity transport in laminar flows encountered in diffuser geometries. The specific objectives of the study include the following:

- Development of a numerical scheme that strictly adheres to the laws of conservation of mass and momentum.
- Providing computational stability over a wide range of time steps.
- Ensuring invariance with respect to the choice of coordinate system; and
- Validating the scheme by comparing it with analytical solutions and classical methods.
- Validation of the scheme by comparison with analytical solutions and classical methods.
- Demonstrating the practical applicability of the scheme to two-dimensional (2D) and three-dimensional (3D) problems.

1.5. Research Questions

This study addresses the following key questions:

1. Can a finite-difference scheme be developed that maintains perfect conservativity, even in the presence of variable velocity fields with sign changes?

2. What advantages and disadvantages does the proposed scheme have over classical methods in terms of accuracy, stability, and computational efficiency?

3. What is the practical significance of conservativity preservation for engineering calculations involving matter flows in diffusers and confusers?

4. How can the new scheme be integrated into existing computational frameworks with minimal changes to the algorithms?

To address these challenges, we must examine current research on finite-difference schemes. Particular attention should be paid to the ability of classical schemes to fulfill the critical properties described in the introduction. Therefore, conservativity, stability, transportability, adequacy, and invariance were key aspects in conducting the literature review of computational schemes.

2. Literature Review

2.1. Finite-Difference Schemes in Computational Fluid Dynamics

For many years, reliable finite-difference schemes for fluid flow calculations have been a key focus in computational fluid dynamics. This section reviews the theoretical foundations and practical approaches related to the five essential properties of numerical schemes mentioned in the introduction. It emphasizes the need for a new numerical scheme. The new scheme aims to address the problems of classical methods, such as the Courant-Isaacson-Rees scheme.

Creating reliable finite-difference schemes has been essential in computational fluid dynamics for decades. Roache emphasized the critical importance of verification and validation in computational fluid mechanics. He noted that many schemes appear promising but fail in practice. This often occurs because they violate basic conservation principles.

Classical finite-difference schemes have been well-studied. They have been categorized based on their key properties. Godunov and Ryabenky [1] provided a comprehensive analysis of difference schemes, establishing the theoretical foundation for stability analysis. The Courant–Friedrichs–Lewy condition is essential. It states that numerical data cannot move faster than the actual speed of transport processes.

Lax and Richtmyer [2] did pioneering work on the stability of linear finite difference equations. Their criteria still influence modern scheme development. They demonstrated that stability alone is insufficient for practical applications because schemes must also possess critical properties, such as conservativity and transportability.

In approximate calculations of aerohydrodynamic problems, the obtained solutions must fulfill the following properties: stability, transportability, conservativity, adequacy, and invariance. If even one of these properties is not met, the result can only serve as an estimate and is rarely sufficient for practical use. Small deviations may allow for approximate use, but large deviations render solutions unsuitable for practical applications.

We will describe the manifestation of these properties by referring to the studies of hydrodynamicists [3, 4].

Stability refers to the formation of a solution that remains unchanged over time when boundary conditions remain constant. The method of establishment [5] yields balanced solutions that are independent of time and initial conditions. This property supports theorems of uniqueness and existence in gas hydrodynamics models [5, 6]. Many schemes can produce stable solutions, including Courant's, the "leap-frog" scheme, the Dufort-Frankel scheme, the Abarbanel-Tsvas scheme, the Lax scheme, the Lax-Wendroff scheme, the Leith scheme, the Nagel scheme, the Godunov scheme, the Arakawa scheme, the Roberts-Weiss scheme, the Crowley scheme, and their modifications [1-4]. These schemes are conditionally stable, subject to constraints such as the Courant-Levy parameter [1, 3, 7-9].

Transportability is the ability to move calculated characteristics only along the flow. This property is peculiar to non-symmetric schemes. Downstream-directed schemes, such as the Levevre scheme, are considered inadequate for practical calculations [10].

Adequacy is a scheme's ability to accurately describe real processes. Inadequate schemes may be discussed in the literature, but they are irrelevant for practical applications.

Conservativity guarantees that the integral laws of conservation in the governing equations are fully met [11, 12]. The Courant-Isaacson-Rees scheme and its modifications possess this property under certain conditions [3, 4]. However, conservativity may be compromised in areas with changing velocity signs [13, 14].

Invariance guarantees independence from the arbitrary choice of coordinate axes. Its absence is evident in the Ranchel scheme, where the influence of neighboring nodes depends on direction [3].

To quote Roache once again: "One of the surprising aspects of computational fluid dynamics is the existence of more plausible schemes that, however, do not work" (1). Some schemes work well in specific situations.

However, none of the schemes meet all five key CFD requirements: conservativity, stability, transportability, adequacy, and invariance.

Excluding symmetric schemes and those that rely on artificial viscosity or second spatial derivatives significantly narrows the number of suitable schemes. The Courant-Isaacson-Rees scheme is the closest known to fulfilling all these requirements.

2.2. Conservative Schemes and Mass Transport

Conservativity is a vital property in physical modeling. Samarskii and Vabishchevich [8] and Samarskii and Vabishchevich [9] developed robust numerical methods for convection-diffusion problems and emphasized the importance of conservation laws.

Pavelchuk and Maslovskaya [10] described modifications to conservative finite-difference schemes for convection-reaction-diffusion problems and noted that traditional schemes perform poorly under complex flow conditions with changing velocity signs.

Salokhiddinov et al. [13] demonstrated that the Courant-Isaacson-Rees scheme experiences conservativity losses in quasi-one-dimensional flows. This emphasizes the necessity of alternatives that maintain conservation under all conditions.

2.3. Transport Phenomena in Diffuser and Confuser Geometries

Recent research has significantly advanced our understanding of transport phenomena in diffuser and confuser geometries, particularly with regard to hydrodynamics and heat transfer. Pakhomov and Terekhov [15] demonstrated that longitudinal pressure gradients substantially influence flow structure and thermal characteristics. Specifically, decreasing angles in confusers leads to the significant suppression of turbulence and reduction of recirculation zones. Conversely, increasing opening angles in diffusers promotes the growth of turbulent kinetic energy and extends recirculation regions. Dyachenko [16] confirmed that increased longitudinal pressure gradients enhance maximum Nusselt numbers in confusers and reduce them in diffusers. These findings provide crucial insights for optimal thermal and flow design strategies.

Complementing these hydrodynamic studies, geometric optimization investigations have been conducted to enhance flow performance. Osipov [17] conducted extensive experimental and theoretical research on direct-flow channel geometries used in hydrogenerators. His work identified optimal contraction angles (30–35°) and expansion angles (7–8°). These angles ensure maximum throughput and efficient flow energy conversion. Vladimirovich expanded this research by examining heat pipes with confuser-diffuser channels. He revealed that optimized geometry and controlled vapor swirl can significantly increase heat transfer coefficients while reducing hydraulic losses, particularly at specific swirl angles.

Studies of diffuser performance in aeration systems have also focused on mass transfer processes, particularly oxygen transfer. Cruz et al. [18] investigated fine-pore diffuser aerators and demonstrated that smaller pore sizes generate fine bubbles, which enhance gas–liquid contact and increase oxygen transfer rates.

However, they also noted that increased efficiency may be offset by greater hydraulic resistance when using a large number or size of openings. Herrmann-Heber et al. [19] conducted in-depth experimental research on micro-perforated diffusers to explore this subject further. They demonstrated that, compared to traditional alternatives, these designs can produce mass transfer coefficients that are up to 270% higher. Similarly, Ham et al. [20] found that fine-pore and micro-perforated diffusers consistently provide higher oxygen transfer efficiency after comparing different diffuser types in bubble columns and airlift reactors. They underlined how crucial it is to take fouling and aging effects into consideration when evaluating the long-term performance of a system.

2.4. Verification and Validation in CFD

Strict verification and validation (V&V) procedures are essential to modern computational fluid dynamics (CFD) in order to guarantee numerical accuracy and physical relevance. Standard V&V methodologies were established by Oberkampf and Trucano [21], which also made a clear distinction between validation, which compares with experimental data while taking into account all sources of uncertainty and verification, which concentrates on detecting and minimizing numerical errors.

Recent research has shown how these ideas are applied in a variety of engineering domains. Chen [22], for instance, used thorough V&V procedures in their CFD simulations of wind turbines. The significance of grid convergence studies and methodical comparisons with experimental benchmarks was highlighted by their findings. Descamps et al. [23] created thorough V&V strategies for ship hydrodynamics in the interim. Their methodology placed a strong emphasis on the necessity of high-resolution grid refinement, time step sensitivity, and the significant computational resources needed to produce reliable results. Collectively, these initiatives highlight the necessity of robust validation frameworks to enhance trust in simulation results across various CFD applications.

2.5. Turbulent Transport and Advanced Modeling

Given its significance in both industrial and natural flows, a thorough understanding of turbulent transport is crucial for the advancement of fluid dynamics. By examining turbulent energy cascades, Alexakis and Biferale [24] made important advances in this area. They exposed intricate patterns in the movement of energy and invariants at various scales, such as situations with several, disjointed, or even two-way cascades. Both localized transport mechanisms and global flow characteristics are shaped by these dynamics.

Data-driven techniques have been incorporated into turbulence research due to recent developments in computational techniques. Results from machine learning, in particular, have been encouraging. Srinivasan et al. [25], for example, showed that deep neural networks can successfully predict turbulent shear flow features, demonstrating good agreement with high-fidelity simulation data. Similar to this, Pandey et al. [26] investigated incorporating machine learning methods into frameworks for turbulence modeling, indicating that these hybrid approaches might be able to overcome the drawbacks of conventional models. These advancements open the door for CFD simulations to capture turbulence complexities more accurately and efficiently.

2.6. Current Limitations and Emerging Challenges

Conservativity remains an issue in non-uniform velocity fields, despite advancements. Under practical circumstances, schemes such as the Courant-Isaacson-Rees method perform poorly. It is also challenging to incorporate new schemes into outdated CFD software.

A review of the literature reveals that the fundamental problem of conservativity under realistic flow conditions has not been solved, despite notable advancements in modeling transport phenomena and in verification and validation procedures. These results highlight the need for a new finite-difference scheme that can be readily incorporated into current CFD frameworks with little computational overhead and guarantees of stability, transportability, conservativity, adequacy, and invariance. This crucial gap is intended to be filled by the suggested strategy, which will be discussed in the sections that follow.

3. Materials and Methods

This study employs a methodical approach that includes theoretical formulation, numerical verification, and empirical testing. The approach consists of: (1) a theoretical development of the conservative finite-difference scheme grounded in basic conservation principles, (2) numerical verification against benchmark problems and analytical solutions, (3) application to real-world diffuser flow problems; (4) comparison with the Courant-Isaacson-Rees scheme and other classical techniques; and (5) evaluation of stability and computational efficiency.

3.1. Research Methodology

Let us construct a scheme for calculating the transport of a conservative impurity on the basis of the mass conservation Equation 1 written for some conservative substance "S" transported at a velocity.

Without diffusion terms in the impurity transport equation, it appears as written in expression (1)

$$\frac{\partial S}{\partial t} = -div\vec{V}S = -\left(\vec{V} grad\ S + S\ div\ \vec{V}\right) \quad (1)$$

Expanded expression (1) is written by expression (2)

$$\frac{\partial S}{\partial t} = -\left[\frac{\partial SV_x}{\partial x} + \frac{\partial SV_y}{\partial y} + \frac{\partial SV_z}{\partial z}\right] = -\left[\left(V_x\frac{\partial S}{\partial x} + S\frac{\partial V_x}{\partial x}\right) + \left(V_y\frac{\partial S}{\partial y} + S\frac{\partial V_y}{\partial y}\right) + \left(V_z\frac{\partial S}{\partial z} + S\frac{\partial V_z}{\partial z}\right)\right] \quad (2)$$

Where V (with projections on the coordinate axes V_x, V_y) is the vector of medium motion, transporting impurity S.

Due to the laminar motion of the medium transporting the impurity, the exact solution will be a complete coincidence of concentrations at the inlet and outlet of the calculation area. Thus, it will be possible to check the accuracy and adequacy of the studied calculation schemes.

For the calculation of multidimensional problems, the method of coordinate splitting is known and widely used [5, 6]. But it is not fundamental and was done only for simplicity of analysis and comparison of solutions, since all solved schemes were solved explicitly. This means that during half of each computational time interval, the processes consistently run along one coordinate axis and then switch to the other axis.

This method makes it possible to simplify the writing of calculation schemes by considering, and sometimes by sequentially calculating, one-dimensional schemes. However, it should be remembered that the schemes are applied in full analogy and for each dimension.

So along the axis OX (index i), we will write down for the component the scheme TIIAME NRU (3) [13, 14] and the scheme (4) "Courant-Isaacson-Rees" [3]:

$$\frac{S^{t+1}_{i,j,k}-S^t_{i,j,k}}{\Delta t} + \left(U_{i,j}\frac{S^t_{i,j,k}-S^t_{i-1,j,k}}{\Delta x} + S^t_{i,j,k}\frac{U_{i+1,j,k}-U_{i,j,k}}{\Delta x} + W_{i,j,k}\frac{S^t_{i+1,j,k}-S^t_{i,j,k}}{\Delta x} + S^t_{i,j,k}\frac{W_{i,j,k}-W_{i-1,j,k}}{\Delta x}\right) = 0 \quad (3)$$

In the formula (3), the parameters $U_{i,j,k} = \max(Vx_{i,j,k}, 0)$, $W_{i,j,k} = \min(Vx_{i,j,k}, 0)$ are calculated.

$$\begin{cases} \frac{S^{t+1}_{i,j,k}-S^t_{i,j,k}}{\Delta t} + \frac{Vx_{i,j,k}\,S^t_{i,j,k}-Vx_{i-1,j,k}S^t_{i-1,j,k}}{\Delta x} = 0\ ,\ Vx_{i,j,k} > 0 \\ \frac{S^{t+1}_{i,j,k}-S^t_{i,j,k}}{\Delta t} + \frac{Vx_{i+1,j,k}\,S^t_{i+1,j,k}-Vx_{i,j,k}S^t_{i,j,k}}{\Delta x} = 0\ ,\ Vx_{i,j,k} < 0 \end{cases} \quad (4)$$

Where $\Delta x, \Delta t$ are space and time steps, respectively.

Similarly, the transfer scheme is written for the coordinate axis OY (everything is done similarly for the index "j" and the rate and velocity of transfer along the axis 'y' as it was done for the index 'i'). To build a three-dimensional scheme, the same actions are performed, but for the index and the component of the transfer rate along the "z" axis.

3.2. Problem Statements

1) Physical model. The problem of conservative admixture transport in laminar flow of an incompressible or compressible medium inside a diffuser with a variable cross section is considered. The mathematical model is based on the transport equation (without diffusion terms):

$$\frac{\partial(\rho S)}{\partial t} + \nabla\cdot(\rho u S) = 0 \quad (5)$$

where S is the impurity concentration, ρ is the density of the medium, and u is the flow velocity vector. For an incompressible medium $\nabla\cdot u = 0$, for a compressible medium $\nabla\cdot(\rho u) = 0$.

2) Geometry and grid. The solution domain chosen is a two-dimensional diffuser with axial symmetry.

The inflow and outflow zones have equal width $L_{in} = L_{out}$, the maximum width in the middle part of the region $L_{max} = 3L_{in}$.

For one of the variants of test problems, it is acceptable to narrow the cross-section to $L_{min} = L_{in}/3$ with subsequent expansion.

The computational grid is adopted with the following parameters: in the longitudinal direction, 100 nodes; in the transverse direction, 36 nodes. For axisymmetric problems, cylindrical coordinates (r, z) are used.

3) Boundary conditions. In the inflow (inlet) region, longitudinal velocity u_{in} = 1 m/s, and transverse velocity v = 0.

Impurity concentration S_{in} = 1 g/L in symmetrical zones at a distance from the axis.

In the outflow (outlet) region, longitudinal velocity u_{out} = 1 m/s, and the transverse velocity is determined from the continuity condition. For an incompressible medium, u = 0; for a compressible medium, ρ = const along the current lines.

Lateral boundaries: sliding (symmetric) conditions: $\frac{\partial S}{\partial n} = 0$, v = 0.

4) Initial conditions. Initial impurity concentration $S_{(t=0)}$ = 0 in the whole region except for inflow zones.

The initial velocity field is determined from the stationary solution of the continuity equation.

5) Test problem conditions:

Case 1 (incompressible medium): The flow passes through an expanding diffuser. The task is the conservativity control comparison of the impurity flow at the inlet and outlet.

Case 2 (compressible medium). Longitudinal velocity u = 1 m/s in the whole domain. The transverse velocity is calculated to prevent the flow from detaching from the boundaries.

Case 3 (variable cross section): Flow contraction to L_{min} and expansion to L_{in} are considered. The objective is to evaluate the loss of conservativity of the schemes in areas of abrupt geometry change.

6) Parameters of numerical experiments

The time step is calculated from the Courant parameter: $R_k = \frac{\Delta t}{\Delta x} V_{max} = 1$.

Evaluation criteria are as follows:

- Conservativity (evaluation of the equality of the integral fluxes of impurities at the inlet and outlet);
- Accuracy (evaluated by comparison with the analytical solution (concentration (S) at the outlet coincides with (S_{in}));
- Stability (evaluated by the absence of numerical oscillations in the flow collision zones);

For axisymmetric problems, the transport equation is written in cylindrical coordinates:

$$\frac{\partial(r\rho S)}{\partial t} + \frac{\partial(r\rho u S)}{\partial z} + \frac{\partial(r\rho v S)}{\partial r} = 0 \qquad (6)$$

- Boundary conditions on the axis of symmetry (r = 0): $v = 0$, $\frac{\partial S}{\partial r} = 0$.

4. Results

4.1. Test Problem 1

The flow of an incompressible medium in a two-dimensional region of variable width, symmetric with respect to an axis aligned along the main flow carrying impurities in this region, is considered. The axisymmetric problem is selected to verify the invariance of the schemes. Boundary conditions symmetric with respect to the symmetry axis should yield symmetric approximate solutions within the computational domain.

First, the solution domain with increased width in its central part was considered. Let a flow of any medium with a velocity of 1 meter per second flow through the zone called "inflow" in the entire zone of "inflow." Let the velocity vector defined in the "inflow" zone be parallel to the symmetry axis of the computational domain. In the "outflow" zone, the velocity vector of the medium should also be equal to 1 meter per second. At each cross section, the longitudinal velocities are equal to each other, but they are defined so that the flow of the contaminant-bearing medium is equal to the flow at the "inlet" and "outlet."

The transverse velocities are calculated in such a way that the incompressibility condition for the impurity-carrying medium is satisfied at every point of the calculation domain.

Let the width of the "inflow" zone be equal to the width of the "outflow" zone. The widest part of the computational domain is three times wider than the "inflow" and "outflow" domains.

An impurity with a concentration of 1 g/l enters the flow at the same distance from the symmetry axis. The computational domain contains 36 nodes in the transverse direction and 100 nodes in the longitudinal direction.

The results of the impurity flow calculation are shown in Figure 1.

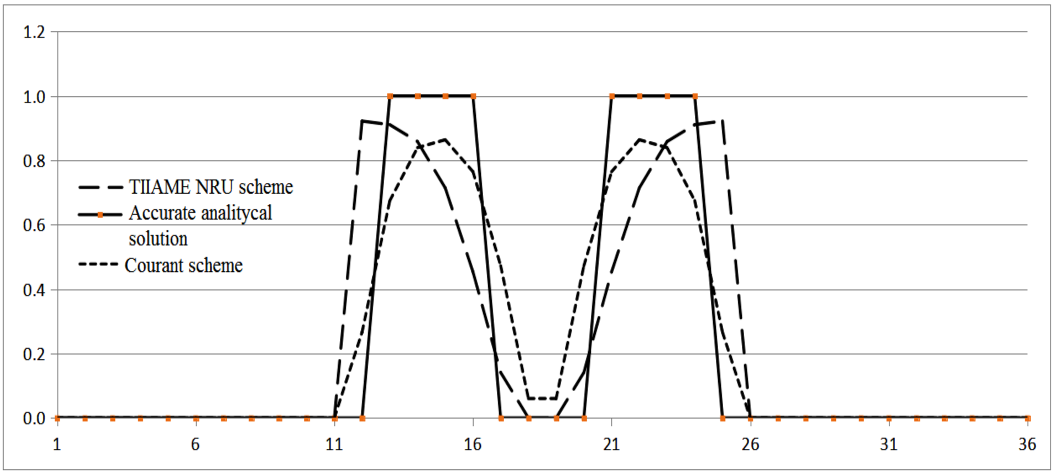

Figure 1.
Calculated impurity flux according to scheme (3) and scheme (4) through successive cross sections of the flow (130th calculation step, R_k = 1).

As shown in Figure 1, the results of the approximate calculation by schemes (3) and (4) are fully conservative and fully coincide in the conservativity characteristics.

The flow velocity slows down in the middle of the computational domain because the medium carrying the impurity is not compressible. As a consequence of this deceleration, one should expect the manifestation of schematic (or computational) viscosity in this domain. Figure 2 shows the exact distribution of the impurity in the output barrel of the solution domain (coinciding with the distribution at the input of the computational domain) and the approximate solution obtained by the Courant-Isaacson-Rees scheme and by the TIIAME NRU scheme [13, 14].

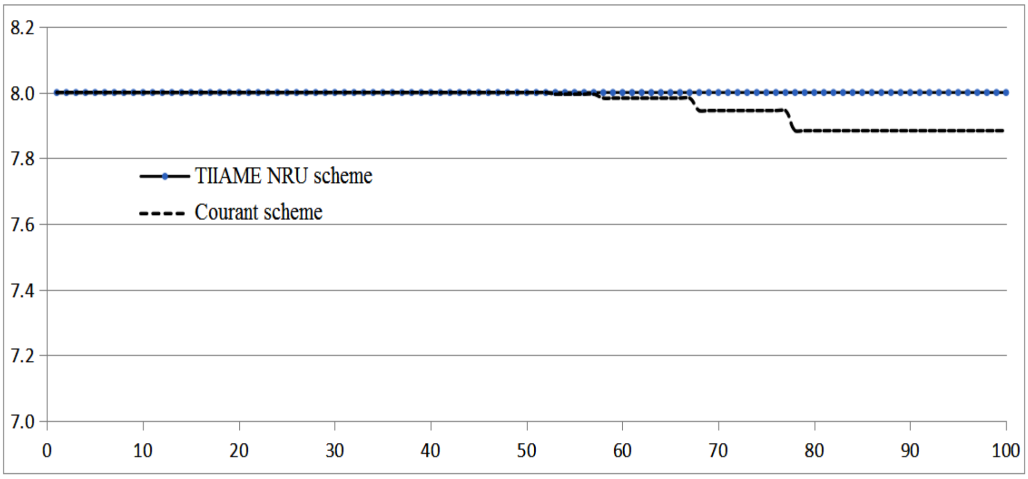

Figure 2.
Comparison of calculations of conservative admixture transport by incompressible medium flow using two different schemes (3) and (4) with the analytical solution.

In Figure 2, we note the manifestation of the scheme viscosity for the approximate solutions obtained by the Courant-Isaacson-Rees scheme and the TIIAME-NRU scheme [13, 14]. The approximate solutions are symmetric, so both schemes are invariant. The Courant-Isaacson-Rees scheme provided an excellent result on the outer sides of the two impurity flows and yielded the same result as the TIIAME NRU scheme on the inner sides of the two impurity flows. We can even say that the Courant scheme performed better than the TIIAME NRU scheme in this case if we do not consider the strange and unexplained pulsation in the impurity streams at their center.

4.2. Test Problem 2

Let us change the condition of the test problem 1. Let the medium carrying the impurity be compressible. Let the longitudinal velocity at each cross section be equal to the inflow velocity of the impurity-carrying medium at the "inlet." Let the longitudinal velocity at each cross section be equal to the inflow velocity of the medium carrying the contaminant at the "inlet." It is quite clear that, in order for the flow not to break away from the edges of the increasing width of the sections and not to cross them as their width decreases, it is necessary to set the transverse velocity appropriately. The medium carrying the impurity loses the property of incompressibility and expands when the computational domain increases and contracts when the computational domain decreases.

Figure 3 shows calculations according to schemes (3) and (4) (TIIAME NRU, Courant et al. [7]) on the distribution of the impurity in the outflow zone, and it also shows the theoretically justified distribution of the impurity as it would result from the exact solution of Equation 1.

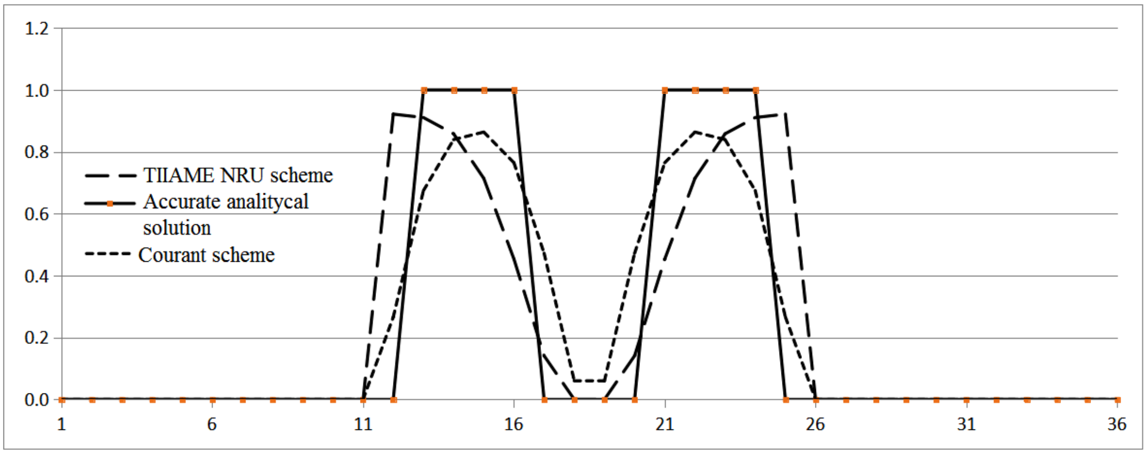

Figure 3.
Comparison of calculations of conservative admixture transport by compressible medium flow according to two different schemes (3) and (4) with analytical solution.

Analyzing the results presented in Figure 3, it is not possible to give preference to any of the schemes studied. Checking the presence of conservativity in the calculations, the loss of conservativity by the "Courant-Isaacson-Rees" scheme is shown in Figure 4.

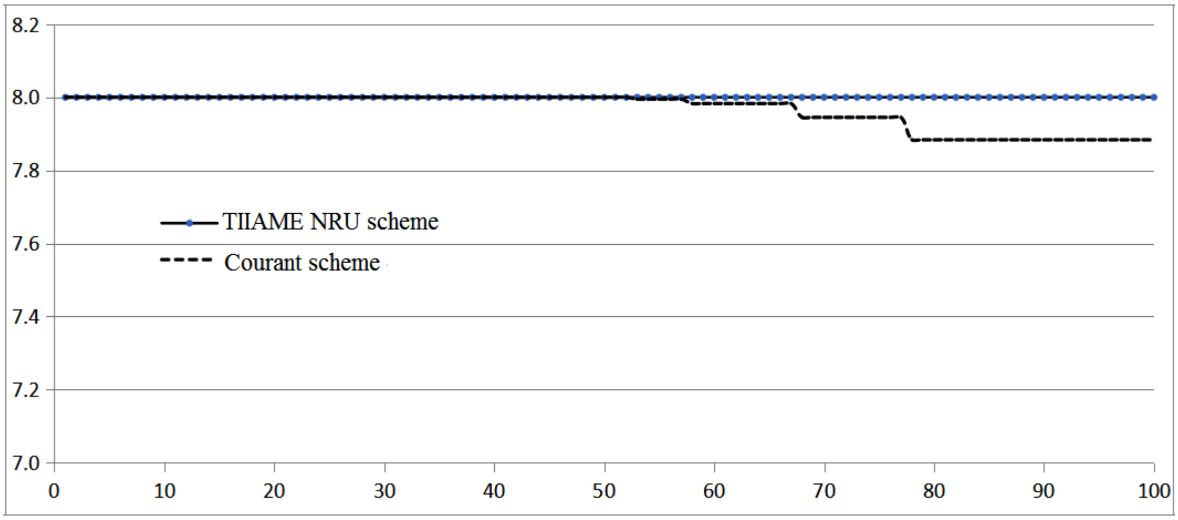

Figure 4.
Calculated impurity flux by scheme (3) and by scheme (4) through successive flow cross sections. The loss of conservativity in the Courant-Isaacson-Rees scheme (4) at flow compression is noticeable.

The loss of conservativity in the Courant-Isaacson-Rees scheme occurred because two impurity streams collided and partially merged at the cross-section reduction section. This results in the loss of conservativity in one-dimensional problems, as shown in Roache [3], Ferziger and Perić [4], Salokhiddinov et al. [13], Savitsky et al. [14] and Savitsky et al. [27], naturally manifests itself in the two-dimensional problem as well.

4.3. Test Problem 3

Consider test problem 3, in which the computational domain is also symmetric as in the previous problem, but the cross section is first reduced by a factor of three and then increased again to the same value.

Again, through the symmetrically arranged zones, the impurity is introduced into the same flow of medium entering and leaving the computational domain as in the previous problem. As can be seen in Figure 5, the Courant-Isaacson-Rees scheme yields the largest expected loss of conservativity in the calculation of impurity transport through incompressible flow.

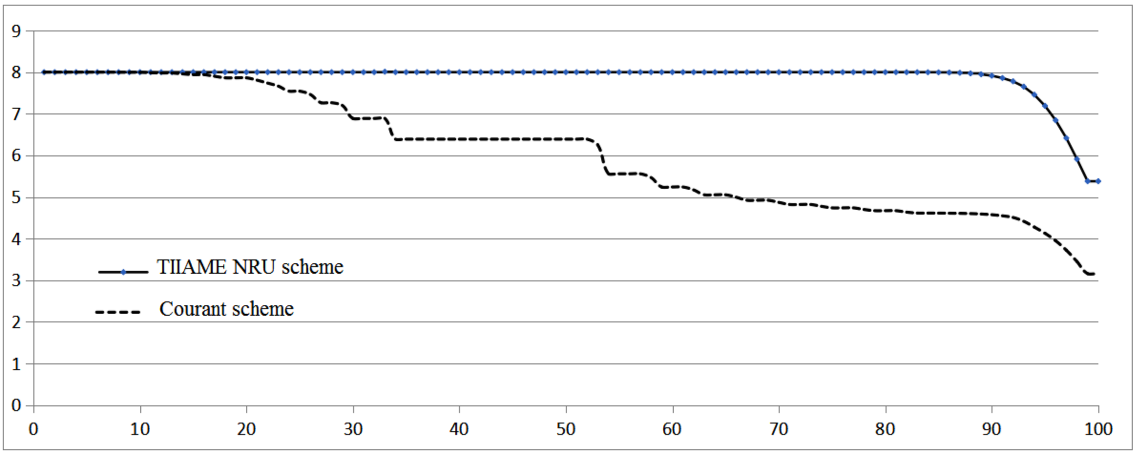

Figure 5.
Comparison of the conservativity property for the TIAME scheme and the Courant-Isaacson-Rees scheme manifested on cross sections of the flow (R_k=1, 190th calculation step). Calculated impurity flux by scheme (3) and by scheme (4) through successive flow cross sections. The computational domain reduces the cross-section and then restores the same value. The medium carrying the impurity is incompressible.

In the right part, we observe the front of the impurity motion, which is smoothed by the viscosity scheme in schemes (3) and (4).

Let us compare the obtained solutions of the TIIAME NRU and Courant-Isaacson-Rees schemes with the exact solution on the cross section equal to the zone of admittance of the impurity into the calculation domain. The comparison of the calculations is shown in Figure 6.

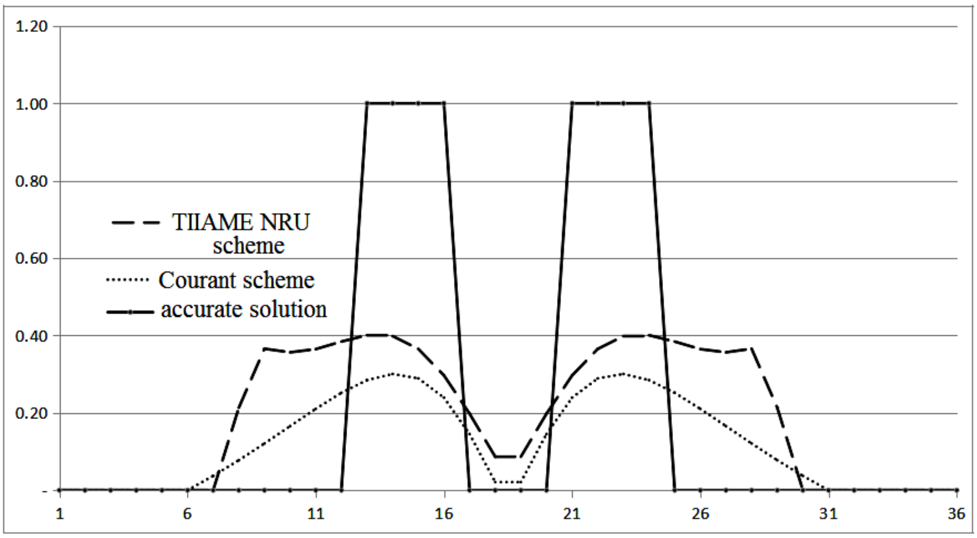

Figure 6.
Comparison of calculations of conservative impurity transport by incompressible medium flow by two schemes (3) and (4) with exact analytical solution at R_k=1, 190th calculation step.

In Figure 6, a strong influence of the scheme viscosity on the approximate solution can be observed. It should be recalled that in the central part of the domain, the velocities reach a value of 3 meters per second, and therefore, the Courant number is much less than 1 in most of the domain. The manifestation of the scheme's viscosity and the fight against it is not the subject of this paper. It is only important that the Courant scheme (3) has lost conservativity, while the TIIAME NRU scheme (4) has retained it.

4.4. Test Problem 4

If we solve the previous problem but under the assumption that the medium is compressible, the approximate solution will agree much better with the exact solution. Let us set the compressibility of the medium carrying the contaminant as follows. The longitudinal velocity of the medium carrying the contaminant is set to 1 m/s everywhere. The transverse velocity of the medium is set so that the medium flow does not cross the lateral boundary of the computational domain and does not break away from it. The results are shown in Figures 7 and 8.

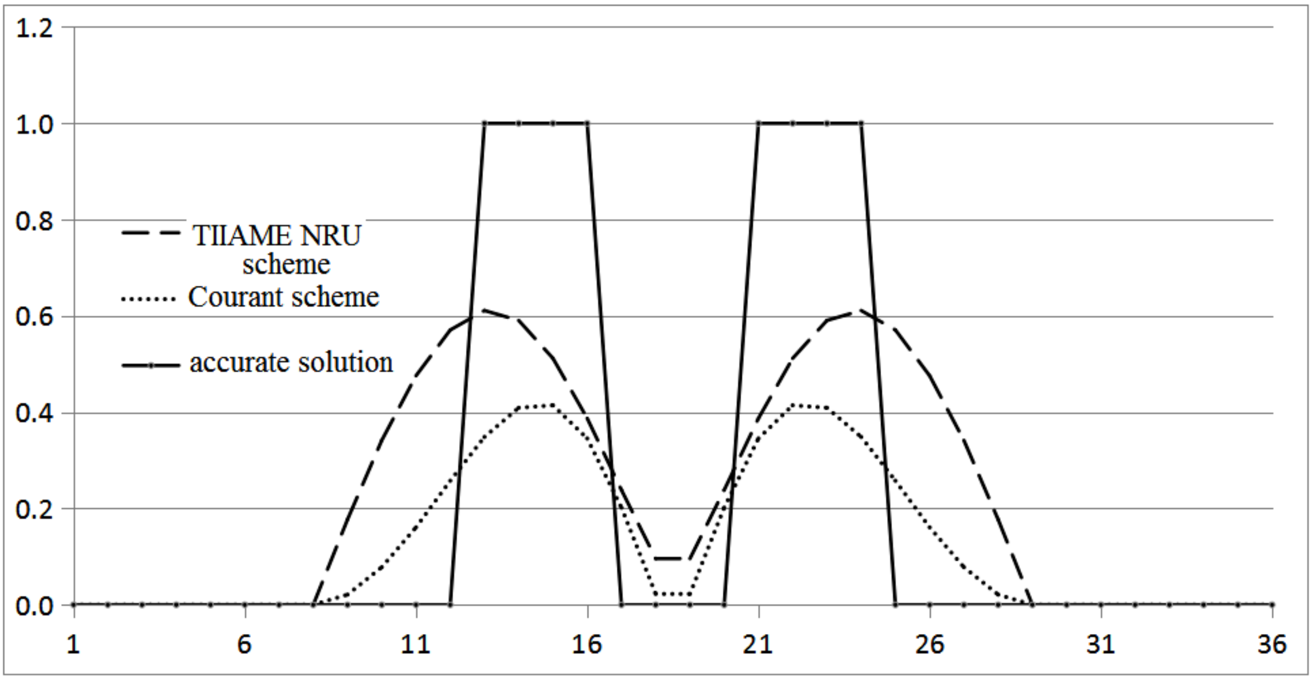

Figure 7.
Comparison of calculations of conservative impurity transfer by the flow of compressible medium according to schemes (3) and (4) with the exact analytical solution at R_k=1, 190th calculation step.

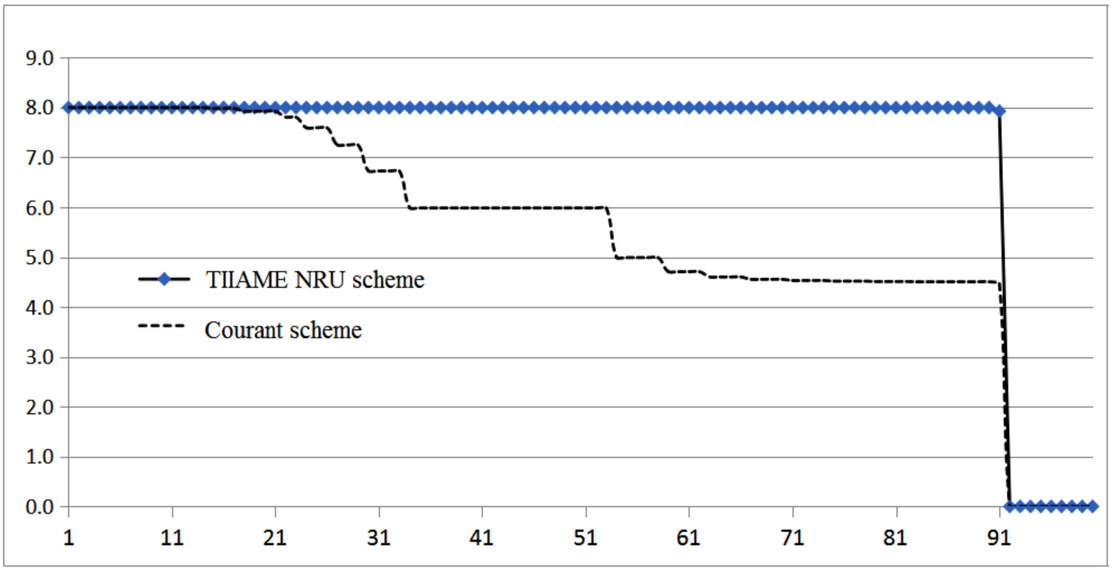

Figure 8.
Calculated impurity flow by scheme (3) and by scheme (4) through successive flow cross sections. Comparison of the conservativity property for the TIAME scheme and the Courant-Isaacson-Rees scheme as manifested on the flow cross sections (R_k=1, 190th calculation step). The computational domain reduces the cross-section and then restores the same value. The medium carrying the impurity is assumed to be compressible.

The analysis of the solutions obtained shows that the TIIAME-NRU scheme is preferable to the Courant-Isaacson-Rees scheme. The main advantage of the TIIAME-NRU scheme is its robust conservativity. The TIIAME-NRU scheme is transportable, computationally stable, adequate, and invariant.

In the transverse direction, the scheme viscosity is significant for schemes (3) and (4) (see Figure 7).

In Figure 8, we see a very weak manifestation of the scheme viscosity in the longitudinal direction. The front of the impurity motion is well expressed.

4.5. Generalization of the TIIAME NRU Scheme to Three-Dimensional Space

Let us consider the possibility of generalizing the TIIAME NRU scheme to three-dimensional space.

First, note that there is no difficulty at all in generalizing to three-dimensional Cartesian space. Similarly, as the scheme (3) written for one-dimensional space was extended to two-dimensional space, it can be generalized to three-dimensional space just as easily. The analogy is complete. It is an entirely different matter when computers deal with pseudo-three-dimensional space or cylindrical coordinates, where the process is symmetric about some axis of symmetry. In fact, the longitudinal and radial velocities of matter are being calculated. It is common to use cylindrical coordinates to calculate processes in which there is no rotation about the axis of symmetry (tangential velocity) to save computation time. In fact, the solution in the three-dimensional domain is determined in the calculation of a plane problem. Therefore, such a calculation can be called a calculation in pseudo-three-dimensional space.

It is understood that there is no rotation about the central axis of symmetry, i.e.,$V_\theta = 0$.

In cylindrical coordinates, Equation 2 takes the form of sentence (7)

$$\frac{\partial S}{\partial t} + \frac{\partial S V_x}{\partial x} + \frac{\partial\, r\, S V_r}{r\, \partial r} + \frac{\partial\, S V_\theta}{r\, \partial \theta} = 0 \qquad (7)$$

where r is the distance to the axis of symmetry. The line with the coordinate $r=0$ is the axis of symmetry, V_x, V_r, V_θ are longitudinal, radial, and tangential velocities of the medium.

Writing down the conservation equation in the form (7) is not yet suitable for assembling a calculation scheme possessing conservativity, and therefore, some identical transformations will be necessary.

Consequently, Equation 7 is simplified to the form (8):

$$\frac{\partial S}{\partial t} + \frac{\partial S V_x}{\partial x} + \frac{\partial\, r\, S V_r}{r\, \partial r} = 0 \qquad (8)$$

Using the rules of differentiation of the product of functions, we obtain the notation (9):

$$\frac{\partial S}{\partial t} + \left(\frac{\partial S V_x}{\partial x}\right) + \left(\frac{\partial\, S V_r}{\partial r}\right) + \frac{S V_r}{r} = \frac{\partial S}{\partial t} + \left(S\frac{\partial V_x}{\partial x} + V_x\frac{\partial S}{\partial x}\right) + \left(S\frac{\partial\, V_r}{\partial r} + V_r\frac{\partial\, S}{\partial r}\right) + \frac{S V_r}{r} = 0 \quad (9)$$

For the first summand, which interacts with the second and third summands (highlighted by brackets), we apply the TIIAME NRU scheme (3).

The fourth summand $\frac{S V_r}{r}$ should be taken into account by a balanced consideration of impurity transport along the radius axis of the symmetric solution domain. The only thing to keep in mind is that the symmetry axis of the solution domain itself is the line of singularity where Equation 9 will cease to exist. Therefore, all calculations will exclude the axis of symmetry by deviating from it by one step of the finite difference grid. Alternatively, we will have to assume that the symmetry axis runs halfway between the two nodes closest to it. In this way, it will be possible to avoid division by zero in Equation 9.

Let us repeat the recording of the developed scheme TIIAME NRU [13, 14] for the form of recording the equation of conservation of impurity (1), considering, for simplicity of recording, only the component of the vector of motion of the medium along the radius axis (distance from the axis of symmetry), but taking into account the summand appearing in the case of application of cylindrical coordinates.

$$\frac{S^{t+1}_{i,r}-S^t_{i,r}}{\Delta t} + \left(U_{i,r}\frac{S^t_{i,r}-S^t_{i-1,r}}{\Delta r} + S^t_{i,r}\frac{U_{i+1,r}-U_{i,r}}{\Delta r} + W_{i,r}\frac{S^t_{i+1}-S^t_{i}}{\Delta r} + S^t_{i,r}\frac{W_{i,r}-W_{i-1,r}}{\Delta r}\right) + \left(\frac{S^t_{i,r}(U_{i,r}-W_{\ i,r})}{r_i} - \frac{S^t_{i-1,r}U_{i-1,r}}{r_{i-1}} + \frac{S^t_{i+1,r}W_{i+1,r}}{r_{i+1}}\right) = 0$$
(10)

In formula (10), $U_{i,r} = \max\left(Vr_{i,r}, 0\right)$, $W_{\ i,r} = \min$ ($Vr_{i,r}$, 0, $Vr_{i,r}$ is the lattice analog of V_r; $U_{i,r}$ and $W_{i,r}$ are temporarily created intermediate variables.

Note that at very large distances from the axis of symmetry and the actual approximation of cylindrical coordinates to Cartesian coordinates, all summands involving division by the value of the distance from the axis of symmetry *r* will disappear. Scheme (10) begins to transform into scheme (3).

The TIIAME NRU scheme can be expressed in cylindrical coordinates while maintaining all its positive properties. This expands its potential for solving the most significant problems in aero-hydrodynamics.

5. Discussion

Numerical experiments have demonstrated that both investigated schemes (TIIAME NRU and Courant-Isaacson-Rees) exhibit acceptable accuracy when applied to flows with simple geometry. However, significant differences arise when the geometry becomes more complex, particularly in zones with variable cross-sections. The TIIAME NRU scheme retains high accuracy in conserving impurity mass even under substantial modifications to the flow cross-section, which aligns with findings from recent studies on conservative numerical schemes [24, 28].

When impurity flows collide, the TIIAME NRU scheme remains stable, whereas the Courant-Isaacson-Rees scheme exhibits numerical oscillations. This behavior has been corroborated by research highlighting the limitations of classical schemes in handling discontinuities and sharp gradients in multi-dimensional problems [29]. A study of the effect of the Courant number on solution accuracy revealed that the TIIAME NRU scheme outperforms the Courant-Isaacson-Rees scheme:

- The TIIAME NRU scheme remains stable when $Rk \leq 1$.
- Optimal results are obtained when $0.8 \leq Rk \leq 0.95$.
- When $Rk < 0.5$, excessive numerical viscosity is observed.
- The Courant-Isaacson-Rees scheme requires a tighter constraint: $Rk \leq 0.85$.
- The manifestation of scheme viscosity differs between the two approaches:
- In the TIIAME NRU scheme, the effect of scheme viscosity is more uniform and predictable.
- The Courant-Isaacson-Rees scheme exhibits local maxima of scheme viscosity in zones of flow direction change.
- At nodes located on the line of symmetry (with zero transverse velocity), the Courant-Isaacson-Rees scheme does not operate effectively in the transverse direction by definition (see formula (4)).

Recent studies on turbulence modeling and computational fluid dynamics (CFD) validation emphasize the importance of robustness and stability in numerical schemes, particularly for applications involving compressible and incompressible flows [21, 22]. These studies highlight that schemes like TIIAME NRU, which maintain conservation laws across diverse velocity configurations, are critical for accurate simulations of multiphase and chemically reacting flows.

Furthermore, contradictory findings from experimental studies suggest that while classical schemes like Courant-Isaacson-Rees may perform adequately in laminar flows, they often fail in turbulent or highly compressible regimes [29]. This underscores the need for advanced schemes such as TIIAME NRU, which can be generalized to three-dimensional space and adapted for cylindrical coordinates [13].

6. Conclusion

6.1. Implications

The study emphasizes the importance of conservativity in computational fluid dynamics (CFD), particularly in two- and three-dimensional aero-hydrodynamics problems. The TIIAME NRU scheme demonstrates reliable performance in conserving mass and momentum, making it suitable for applications in jet engine nozzles, gas burners, and thermal power plants. Its capacity to handle both compressible and incompressible flows ensures its relevance across a broad spectrum of engineering challenges [15, 16].

6.2. Limitations

Despite its advantages, the TIIAME NRU scheme has certain limitations:

- It requires 15–20% more computational resources due to the calculation of intermediate parameters.
- Boundary conditions must be carefully formulated to ensure conservation laws are satisfied at the domain boundaries.
- The scheme's performance may degrade in cases where grid resolution is insufficient or time steps exceed optimal values [30].

6.3. Future Research Suggestions

Further research can focus on the following directions:

1. Generalizing the TIIAME NRU scheme for pseudo-three-dimensional problems in cylindrical coordinates could enhance its utility in axisymmetric regions such as combustion chambers and nozzles [31].
2. Conducting rigorous verification and validation (V&V) studies using high-fidelity experimental data will strengthen confidence in the scheme's predictions [30, 32, 33].
3. Exploring machine learning techniques to optimize grid refinement and reduce computational costs could further improve efficiency [25, 26].
4. Investigating the scheme's performance in multiphase flows with phase transitions could expand its applicability to industrial processes such as aeration systems and bubble column reactors [19, 20].

6.4. Comparative Analysis of Schemes

To summarize the key differences between the investigated schemes (TIIAME NRU and Courant-Isaacson-Rees), the following comparative table highlights their recommended application areas, limitations, and performance characteristics:

Table 1.
Comparative conclusions on the calculation schemes.

	TIIAME NRU scheme	**Courant-Isaacson-Rees scheme**
Recommended application area	• Calculation of flows with strong geometry changes • Presence of zones with velocity sign change at boundaries • Calculation of chemically reacting flows • Modeling of multiphase flows, where the number of phases moving together and possible phase transitions are of particular importance. • Accuracy is of fundamental importance and influences the solution. • Cases when computational accuracy in the laws of conservation of mass and momentum is important	• Simple flows without significant change of geometry • Small number of zones with a change of velocity sign on the boundaries • The simplest cases of transfer of one or several phases without considering phase transitions. • Accuracy is not of fundamental importance and does not influence the solution. • Cases where computational accuracy is not important in the laws of conservation of mass and momentum.
Limitations of applicability	• Several increased demands on computational resources • Boundary conditions must be written in such a way as to ensure the fulfillment of conservation laws at the boundaries of the computational domain.	• Some computational problems with the calculation of transport at zero velocities, such as at axes of symmetry in the computational domain and for transverse transport velocities. • Loss of conservativity in some cases.

This table underscores the strengths and weaknesses of each scheme, providing a clear guideline for their practical implementation in various engineering scenarios.

By addressing these areas, future work can build on the strengths of the TIIAME NRU scheme while mitigating its limitations, contributing to advancements in computational fluid dynamics and its practical applications.

The issue of loss of conservativity is among the most significant problems in computational fluid dynamics. The paper demonstrates that situations with velocity configurations leading to the loss of conservativity in the most well-known transport schemes are almost always encountered in two- and three-dimensional problems of aero hydrodynamics. Conservativity is particularly crucial in cases where multiple types of contaminants interact, transporting and potentially forming a separate medium that carries them through space. These include jet engine nozzles, gas burners, and boilers in thermal power plants, where a dispersed mixture of several components is burned in air jets, and directed convergent plasma flows are created for either destruction or creation.

The precise calculation of the quantities of interacting components carried in the medium is of practical interest only if the conservation laws are strictly observed. The TIIAME NRU scheme allows the conservation laws to be observed in different velocity configurations and is applicable to both incompressible media and compressible media flows carrying an impurity. Its widespread use in aerodynamic and hydrodynamic problems is expected and well established.

Only very minor modifications to the code of algorithms of existing mathematical hydromechanical models will be required to completely eliminate the problems associated with the loss of conservativity in conservative contaminant transport calculations.

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