Estimating Scheme Viscosity for Small-Scale Circulation with Implicit Finite-Difference Schemes

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Abstract. The article proposes a formula for calculating scheme viscosity, which manifests itself in calculations using implicit schemes for calculating the transfer of matter and momentum. The study aims to substantiate the structure of the formula for calculating the scheme viscosity using implicit schemes for calculating the mass and momentum transfer equation. As a result of the study, the structure of the formula for calculating the scheme viscosity for implicit schemes for solving the transfer equation was determined. The accuracy of the formula was checked on a test example. It is substantiated that by all possible means, it is necessary to avoid using implicit schemes when solving problems of small-scale circulation within urban areas. The manifestation of scheme viscosity in calculations of small-scale circulation, in which small pressure drops provide air movement, is unacceptable due to the many times the greater effect of scheme viscosity over natural viscosity.

1 Introduction

When solving equations in partial derivatives by the method of finite differences, various algebraic constructions are used, which are analogs of differential terms. These constructions are called finite difference schemes [1]. If, when solving by algebraic methods, the desired characteristic at any point can be determined for this isolated point in the calculated time layer and based on one algebraic equation, then such schemes are called explicit. Suppose the solution can be obtained only by considering all points simultaneously in their relationship on the calculated time interval that is, by solving systems of algebraic equations. In that case, such schemes are called implicit [2].

The solution obtained using finite difference methods is almost always somewhat smoothed (averaged). For example, when solving a simple equation for the transfer of matter, the solution is obtained as if the equation contains terms responsible for the diffusion of matter [3]. Moreover, no such terms exist in writing the equation and its finite-difference analog. Nevertheless, the solution behaves like these terms exist and participate in the calculation. The action of these imaginary terms is called the manifestation of

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artificial computational viscosity or numerical diffusion. The coefficient of this numerical diffusion can be calculated using the well-known formula of computational aerodynamics [2], [4–8].

However, this formula is derived only for explicit finite difference schemes. The method for calculating the circuit's computational viscosity, which manifests itself when using implicit finite-difference schemes, must be developed.

Implicit schemes are widely used in computational tools for various mathematical models of aero and hydrodynamics. Atmospheric circulation models almost always have a computational mechanism based on implicit schemes. This is due to the increased computational stability of implicit calculation schemes. However, what value does the computational viscosity show up in such calculations, and how can it be estimated? This question still needs to be definitively answered. Suppose in large-scale circulation calculations, all parameters of the moving atmosphere are sufficiently smoothed, and the scheme viscosity is not particularly noticeable in the calculations, then for small-scale circulation (the scale of detached buildings). In that case, the scheme viscosity can distort the solution too much. This paper is devoted to the question, "how to estimate the scheme viscosity of the equations of transfer/conservation of matter and energy?".

2 Materials and Methods

Implicit schemes are widely used in computational fluid dynamics. Weather forecasts and the configuration of ocean currents are obtained using implicit calculation schemes for the equations of motion of a continuous medium and the equations of transfer/conservation of matter. But implicit schemes have several disadvantages:

Firstly, economic calculation algorithms (forward and backward sweeps) have been developed only for one-dimensional problems [5,7–12].

Secondly, the results are always very smooth due to the strong manifestation of scheme viscosity [2].

They learned to deal with the first disadvantage. G.I. Marchuk [5,7–9], [13–15] developed a method of coordinate-wise splitting of hydrodynamic problems. The three-dimensional problems were divided into a series of interrelated one-dimensional problems. Thanks to these works, mathematical models for predicting aerodynamic phenomena worldwide began to develop rapidly.

All that is known from the literature [2] about the second drawback of implicit schemes is that this drawback (computational viscosity) always exists and manifests itself very strongly.

The prevalence of implicit schemes in computational aero and hydrodynamics is due to solutions becoming stable. Many scientists have accepted the powerful manifestation of artificial viscosity as an inevitable price for the acquired stability in solutions. It is generally accepted that this strong manifestation of viscosity in implicit schemes is an inevitable evil that cannot be fought and can't be destroyed. The desire to get some solutions to complex multidimensional problems forced the computing practitioners to agree with the most robust "smoothing" of solutions when using implicit schemes [2,4,6–9,13,16–18] etc.

Works combating this "smoothing" phenomenon gave rise to a group of so-called semi-explicit schemes and schemes of higher-order approximations [2,19–26]. But more success has yet to be achieved. The more explicit the scheme was, the more unstable the solutions were; the more implicit the scheme was, the more "viscous" the solutions were.

To estimate the magnitude of the scheme viscosity that arises when calculating the transfer/conservation equations, we will conduct a mathematical analysis, numerical experiments, and do some heuristic studies. Note that the terms that generate the scheme viscosity are also present in the equations of motion (momentum conservation equations). These terms are called not "convective" but inertial terms in these equations. The inertial terms generate the scheme viscosity and lead to the "smearing" of the momentum of motion over the solution region. This once again emphasizes the practical importance of this study.

3 Results and Discussion

To study the manifestation of scheme viscosity in implicit schemes, we consider the simplest equation of conservation/transfer of some substance S in one-dimensional space [6,12,27–29], extending the obtained conclusions to the equation of conservation of momentum.

$$\frac{\partial S}{\partial t}+\frac{\partial(V\cdot S)}{\partial x}=0 \qquad (1)$$

where:
S is some conservative substance,
V is speed is assumed to be constant,
∂ is derivative sign,
t is time,
x is spatial coordinate.
Recall that equation (1) can be written in algebraic form using explicit (2) or implicit (3) finite-difference analogs [2,6,19–21] etc.

$$\frac{{S_o}_{i,j}^{t+1}-{S_o}_{i,j}^{t}}{\Delta t}+V_{i,j}^{t}\cdot\frac{{S_o}_{i,j}^{t}-{S_o}_{i-1,j}^{t}}{\Delta x}=0\ V_{i,j}^{t}>0 \qquad (2)$$

$$\frac{{S_o}_{i,j}^{t+1}-{S_o}_{i,j}^{t}}{\Delta t}+V_{i,j}^{t}\cdot\frac{{S_o}_{i,j}^{t+1}-{S_o}_{i-1,j}^{t+1}}{\Delta x}=0, V_{i,j}^{t}>0, \qquad (3)$$

The analog scheme in the notation (2) and (3) for the spatial derivative is called the "left corner" or the "upstream" scheme. This type of scheme ensures the stability of the solution and the adequacy of the operation of the analog scheme for the term containing the spatial derivative in the impurity transfer/conservation equation (1). The "left corner" scheme should be replaced by the "right corner" scheme if the substance transfer rate becomes a negative value [2,6] etc. This replacement guarantees a stable and adequate Eq. (1) solution at a negative material transfer rate. In addition, the decision must be conservative. The conservativeness of the solution lies in the fact that at each moment, the amount of substance in the calculation area is a constant value if there is no inflow or outflow of substance from the solution area. In "TIIAME" NRU, such a conservative scheme was developed, which exhibits conservatism for any configuration of the velocity fields [30,31]. In the case of a constant speed of the substance (1), the new scheme of "TIIAME" NRU is identical to the most famous scheme of Courant-Isakson-Ries, which, at a constant value of the velocity transfer rate, also coincides with the scheme of Lax Wendroff [2,6,22].

The conservatism of schemes will be tested in all studies of the manifestation of scheme viscosity due to the fundamental importance of this property.

Algebraic equation (2) is an analog of the differential equation (1), which is convenient for mathematical analysis.

As shown in [12], by identical mathematical transformations, the first differential approximation of the difference scheme (2) looks like this:

$$\frac{\partial S}{\partial t}+V\cdot\frac{\partial S}{\partial x}=\left(-\frac{V^2\cdot\Delta t}{2}+\frac{V\cdot\Delta x}{2}\right)\cdot\frac{\partial^2 S}{\partial x^2} \qquad (4)$$

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From the analysis of equation (4), two important conclusions follow:

- The value in brackets can be considered as some artificial viscosity that appeared due to the representation of the differential equation by finite-difference algebraic analogs on the grid function.
- Equation (4) will have a stable and adequate solution only if the value in brackets is not negative.

The second point in the above conclusions follows the rule - "an evolutionary equation with a second spatial derivative is solvable only if the coefficient in front of the second spatial derivative to the right of zero is greater than 0".

It is known and proven by theory and practice that equation (4) has a stable solution only if the coefficient before the second derivative is positive [2,4] and many others. This coefficient is the scheme viscosity coefficient for the explicit scheme.

Equations similar to equation (1) describe diffusion propagation of matter or heat transfer by heat conduction from hot space spots to colder ones. It is clear that the process of collecting heat or matter back to a point from the surrounding space by diffusion is not possible. It is not possible either in nature or in the computational process. An attempt to calculate such a process always leads to an emergency stop of computer technology.

That is, in the computational analog (2) of equation (1), some invisible component μ_a appears, as it were, as defined in the notation (4)

$$\mu_a = \left(\frac{V\cdot\Delta x}{2} - \frac{V^2\cdot\Delta t}{2}\right) \quad (5)$$

and this component μ_a must be greater than zero

$$\left(\frac{V\cdot\Delta x}{2} - \frac{V^2\cdot\Delta t}{2}\right) \geq 0 \quad (6)$$

Equation (6) gives the maximum possible time step value that would provide a stable solution.

$$\Delta t \leq \frac{\Delta x}{V} \quad (7)$$

or

$$1 \leq \frac{\Delta x}{V\cdot\Delta t}, \quad K_0 = \frac{V\cdot\Delta t}{\Delta x} \leq 1 \quad (8)$$

where K_0 is a parameter with a common name - the Courant-Levy parameter [2,6–8] etc. Let's take it out of the bracket $\frac{V\cdot\Delta x}{2}$ in expression (6) as it is usually done [13] and get (9)

$$\mu_a = \frac{V\cdot\Delta x}{2}\cdot\left(1 - \frac{V\cdot\Delta t}{\Delta x}\right) = \frac{V\cdot\Delta x}{2}\cdot(1 - K_0) > 0 \quad (9)$$

From the positivity μ_a it follows that the limiting value K_{max} for the parameter K_0, at which a stable calculation $K_{max}=1$ is possible.

Formula (9) reveals to us the dependence of the scheme viscosity on the chosen value $\frac{V\cdot\Delta t}{\Delta x}$ - the Courant-Levy parameter [6] for the explicit scheme "upstream" [2] etc.

Let's check the accuracy of formula (8) using a test example. The need for such a check is due to the following circumstance. The fact is that when working with approximations of differential equations, practical researchers always add words that there is hope for a close location of the approximate solution and the solution of the original equation. Confidence and hope are not synonymous.

In a one-dimensional space, we construct a grid, the nodes of which are 1 meter apart. Let's set the movement speed of matter equal to 1 meter per second in each grid node. Let us define the substance content everywhere on the spatial axis equal to zero, except for the node point with the number 5. At point 5, we set the substance concentration equal to 10 $[\frac{kg}{m^3}]$. We will consider the solution to the problem for the 50th second.

Let us check the operation of formula (9). To do this, we compare two solutions to the problem of transfer/conservation of matter (1) obtained from the solution of equation (2) using equations (10) and (11), For different values of the Courant parameter K_0.

$$\frac{S_{o_i}^{t+1} - S_{o_i}^{t}}{\Delta t} + V_i^t \cdot \frac{S_{o_i}^{t} - S_{o_{i-1}}^{t}}{\Delta x} = 0, \quad K_0 < 1 \tag{10}$$

$$\frac{S_{o_i}^{t+1} - S_{o_i}^{t}}{\Delta t} + V_i^t \cdot \frac{S_{o_i}^{t} - S_{o_{i-1}}^{t}}{\Delta x} = \mu_s . \frac{S_{o_i}^{t} - 2 \cdot S_{o_i}^{t} - S_{o_{i-1}}^{t}}{\Delta x^2}, \quad K_0 = 1 \tag{11}$$

When solving equation (10), artificial viscosity will manifest. When solving equation (11), there will be no artificial viscosity, but there is a real action of viscosity μ_s, which we will introduce into the calculation and determine its numerical value.

If μ_s is calculated by the formula (9) as a function of K_0, then solutions (10) and (11) will have to coincide for any K_0 of the interval allowed by the Courant Levy condition - $K_0<1$. An example of the coincidence of solutions (10) and (11), after using formula (9), is shown in Figure 1.

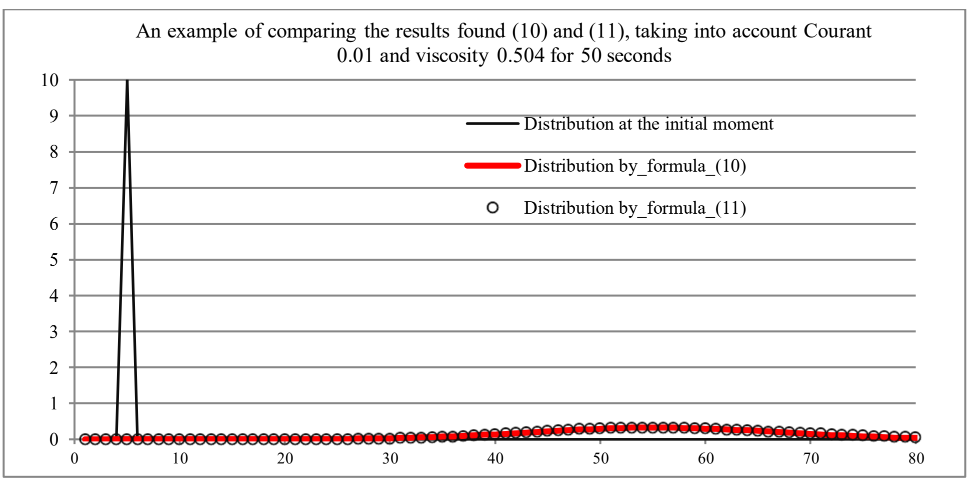

Fig. 1. Example of comparing solution of equations (10) and (11) with Courant number equals 0.01. Coefficient μ_s was selected manually and coincided in value with value calculated by formula (9).

Let us check the assertion about the coincidence of solutions of equations (10) and (11) under the condition that formula (9) is applied. To do this, in Figure 2, we will display: manually selected values μ_s and theoretical values of artificial viscosity for speeds of 1 and 2 meters per second and a set of Courant numbers (0 - 1).

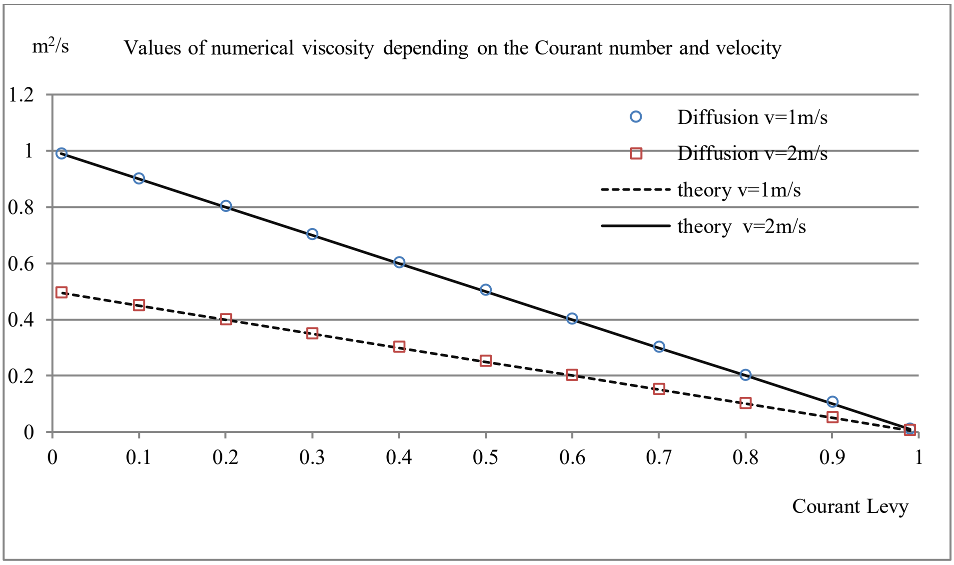

Fig. 2. Manually selected values of viscosity (diffusion) ensuring identity of solutions of equations (10) and (11). Points - calculation with manual selection of viscosity coefficient μ_s. Lines are theoretical values of viscosity (diffusion) calculated by formula (9) for an explicit "upstream" transfer scheme.

Figure 2 proves the high accuracy of equation (9) for calculating artificial viscosity in explicit schemes (2) of the transfer equation (1).
Now let us determine what the scheme viscosity will be if, instead of the explicit scheme (2), the implicit scheme (3) is used to solve equation (1). To evaluate the effect of scheme viscosity manifested in implicit schemes, it is no longer enough to evaluate "very viscous schemes". We need a calculation formula, and it will be offered.
The solution to the implicit scheme (3) can be obtained by forward and backward sweeps [9,14].

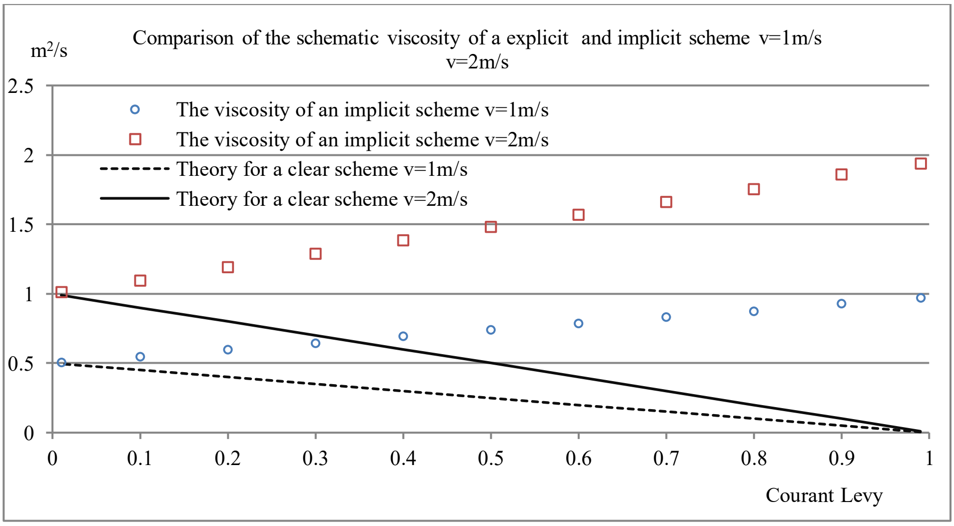

Fig. 3. Comparison of scheme viscosity of explicit and implicit schemes v=1m/s v=2m/s for different values of Courant-Levy parameter and two different values of substance transfer rate.

As for the case of determining the viscosity of the explicit scheme (10), equation (11) was used, in which a value was selected that ensures the equality of solutions, and for the case of the implicit scheme (3), equation (11) was used. Through numerous repetitions, such a value of viscosity μ_s in equation (11) was selected such that the solution of equation (3) coincided with the solution of equation (11).

Figure 3 shows the results of these calculations, together with the theoretical values of artificial viscosity according to formula (9) for explicit schemes. The formula for the scheme (computational) viscosity when using implicit schemes for solving the problem of substance transfer (3) can have the form:

$$\mu_a = \frac{V\cdot\Delta x}{2}\cdot\left(1+\frac{V\cdot\Delta t}{\Delta x}\right) = \frac{V\cdot\Delta x}{2}\cdot(1+K_0) \tag{12}$$

Notably, with an increase in the Courant-Levy number, the scheme viscosity increases when implicit schemes are used. Moreover, the minimum value of the circuit viscosity of implicit circuits is the maximum value of explicit circuits. One can at least try to reduce the scheme viscosity with explicit schemes by increasing the Courant-Levy number. In implicit schemes, the computational viscosity is an indestructible parasitic property of the calculation, and the implicit scheme is always more viscous than the explicit one. The implicit scheme does not lose stability for the Courant-Levy parameter and 10 and 100. But for large values of the Courant-Levy parameter, the solution becomes so viscous that it loses its practical value.

The following fact is about how harmful the manifestation of circuit viscosity can be. The kinematic viscosity of water is $1.7\cdot 10^{-6}\frac{\text{m}^2}{\text{s}}$, and the minimum scheme viscosity when solving the problem of impurity transfer (1) using scheme (3) with water velocities $1\frac{\text{m}}{\text{s}}$ at a grid step of 1 m will be $0.5\frac{\text{m}^2}{s}$. In calculations, the calculated viscosity will exceed the real viscosity thousands of times. Figure 4 shows the solution of the matter transfer equation (1) obtained using the implicit scheme (3) for the Courant-Isakson-Rees pattern for some values of the Courant-Levy parameter. We repeat that the restriction on the Courant-Levy parameter $K_0 < 1$ is removed.

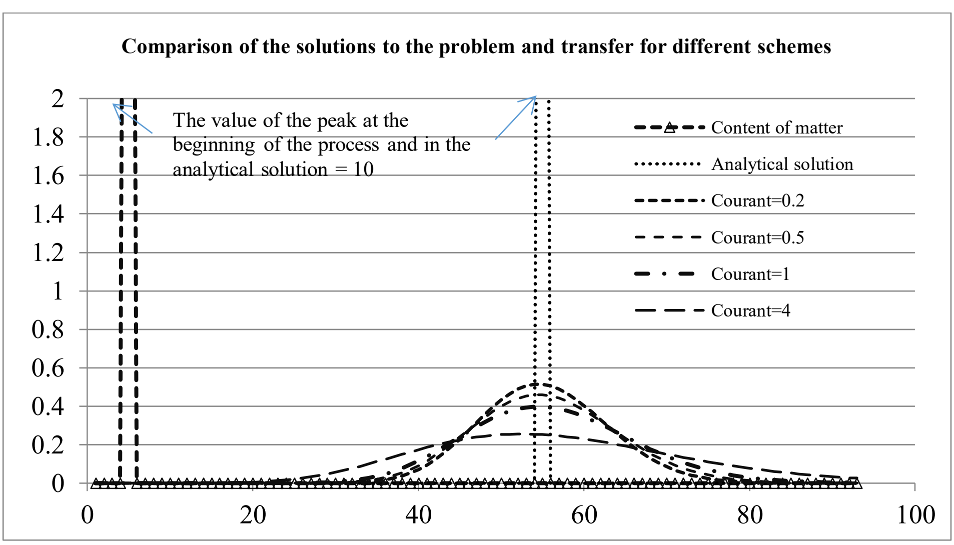

Fig. 4. Comparison of solutions to problem (1) using implicit scheme (3) for series of different values of Courant-Levy parameter.

Let us carry out a mathematical analysis of the first approximation of implicit schemes for the differential equation (1) as it was done for explicit calculation schemes [3]. Mukhin, S.I. et al. [3] use the Taylor series expansion to write expressions for a smooth continuous function of solutions S(t,x) to equation (1) on a grid function in the form of equations (13) and (14)

$$S(t+1,x) = S(t,x) + \sum_{l=1}^{\infty} \frac{\Delta t^l}{l!} \cdot \frac{\partial^l S(t,x)}{(\partial t)^l} \tag{13}$$

$$S(t,x-1) = S(t,x) + \sum_{l=1}^{\infty} (-1)^l \frac{\Delta x^l}{l!} \cdot \frac{\partial^l S(t,x)}{(\partial x)^l} \tag{14}$$

Note that equation (14) can be written as (15)

$$S(t,x) = S(t+1,x) - \sum_{l=1}^{\infty} \frac{\Delta t^l}{l!} \cdot \frac{\partial^l S(t,x)}{(\partial t)^l} \tag{15}$$

Equation (15) is the result of expanding the function for implicit circuits.
This means that if we repeat all the rather long actions published in [3], then in the resulting formula (9) obtained by the authors, the sign in front of the term containing from Δt "-" to "+" will change.
Instead of formula (9)

$$\mu_a = \frac{V \cdot \Delta x}{2} \cdot \left(1 - \frac{V \cdot \Delta t}{\Delta x}\right) = \frac{V \cdot \Delta x}{2} \cdot (1 - K_0) \tag{16}$$

formula (16) will be obtained

$$\mu_a = \frac{V \cdot \Delta x}{2} \cdot \left(1 + \frac{V \cdot \Delta t}{\Delta x}\right) = \frac{V \cdot \Delta x}{2} \cdot (1 + K_0) \tag{17}$$

This is proof that the scheme viscosity arising from the use of implicit calculation schemes of type (3) for solving equation (1) can be calculated using formula (12).

Is it possible that formulas (9) and (12) depend on any other parameters besides the space step, velocity, and the Courant-Levy number? To answer this question, Sedov's π-theorem should be applied. The existence of a regularity, which later received the name of Sedov's π-theorem, was first announced by Bertrand as early as 1878 [19]. To the level of a theorem with variants of use in fluid mechanics, this pattern was developed by Sedov L.I. [32].

The essence of the theorem is as follows. Any pattern in any physical phenomenon is determined by the product of the functions of dimensionless invariants, composed of the parameters that determine this physical phenomenon.

Let us compose dimensionless invariants from the dimensional quantities included in equation (2) or equation (3), which are identical in the set of parameters.

In equations (2) or (3), we have the following dimensions in terms: space step Δx →meter, time step Δt→ sec, $V_{i,j}^t \to \frac{m}{s}$, viscosity $\mu_a \to \frac{m^2}{s}$. Viscosity in equations (2) or (3) is contained invisibly and appears as a consequence of the calculation in finite differences. The value S is, in fact, unique, and it is impossible to compose any dimensionless invariant with it. Therefore, we remove variable S from consideration.

Only the following three dimensionless invariants can be constructed:

Courant number $K_0 \to \frac{V \cdot \Delta t}{\Delta x}, \frac{V \cdot \Delta x}{\mu_a}, \frac{\Delta x \cdot \Delta x}{\mu_a \cdot \Delta t}$.

The third invariant is not independent and can be obtained by dividing the second invariant by the first. Therefore, the third invariant can be removed from consideration.

Since the functions in which this or that invariant participates are not defined, we can directly replace the most interesting function for us, containing the most interesting invariant for us, with the invariant itself.

Then, according to the π-theorem, the equality

$$Const = \frac{V \cdot \Delta x}{\mu_a} \cdot \ \Psi(K_0)$$

The value *Const* is fixed and constant. The graph (3) clearly shows the value *Const*=2. The expression $\Psi(K_0)$ is some function of the Courant-Levy number. The graph (3) clearly shows that this is a linear function $\Psi(K_0) = 1 + K_0$ for the implicit scheme and $\Psi(K_0) = 1 - K_0$ for the explicit scheme. Hence, as suggested above, the formula for calculating the artificial viscosity in the transfer equations when using implicit schemes with high probability looks like (12).

Let us repeat this important result at the end of this article and propose it for the application

$$\mu_a = \frac{V \cdot \Delta x}{2} \cdot (1 + K_0)$$

Using implicit diagrams, the value of schematic viscosity can also be evaluated when using implicitly finished schemes to solve the equations of the substance transfer in the laws of maintaining a mass and the equations of the preservation of a pulse in the equations of movement.

It should be emphasized that the number of chimes when choosing a step in time in implicit schemes ceases to work as a limiting factor. You can choose the number of chimes and 2 and 20! With any values, a stable result will be obtained. Based on the formula (17), viscosity in the resulting result will be prohibitively high. The usefulness and informativeness of this result will be lost. It is enough to look at Figure 4, in which the peak of the analytical solution did not even fit together with the numerical decisions received. If you change the scale and place the peak of an analytical solution on the schedule, then numerical solutions visually merge with the horizontal axis of the coordinates. Therefore, using implicit types of schemes in solving the tasks of the movements of the squat layer of the atmosphere in conditions of small-scale urban development is not advisable due to the loss of information contained in the calculations.

4 Conclusions

When using implicit schemes for calculating the equations of preservation of mass and momentum:

- the restriction on the stability of the solution from the Courant-Levy parameter is removed,
- a schematic viscosity arises and manifests itself, which cannot be destroyed in any way,
- the minimum schematic viscosity when using implicit circuits is equal to the maximum schematic viscosity when applying obvious schemes for the same tasks,
- the size of the schematic viscosity is calculated by the formula (17).

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