NEW METHOD FOR SOLVING THE NAVIER-STOKES EQUATIONS WITH ARTIFICIAL RELATIONS BETWEEN VARIATIONS OF QUANTITIES, APPLIED AT NEAREST NODES

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Abstract. With the use of the Newton method, a new numerical method previously published\(^1\) for solving the three-dimensional Navier-Stokes equations, is theoretically proved for the most simple case of one-dimensional acoustic equations. The convergence of iteration scheme is proved. In this paper, we also recall some theoretical and numerical results presented earlier in\(^1\). The gradient of internal energy (see \(^1\)) has to be redefined. This yielded in\(^1\) that, along with descending temperature of internal walls, some small variations of balance of mass arose within the flow of a gas heated from its motion along tube walls.

The author succeeded\(^1\) in achieving the maximal time step \(\Delta t_{\text{max}} = h/u_{\text{flow}}\) (\(h\) is the average size of cell, \(u_{\text{flow}}\) stands for the flow velocity) along with the condition that, on every step, the required computation time exceeds approximately 6 times the time necessary for computation via an explicit scheme. Every step requires a number of arithmetic operations of order of \(N\); here \(N\) is the number of nodes and cells. The stability and velocity of convergence were estimated in a numerical experience. Satisfactory correlation is obtained between the analytic and computed balances of mass in a tube for a given wall temperature dependence.

Next, briefly, the idea of the method includes an artificial binding of unknowns' corrections at neighbouring nodes or cells; the respective corrections are determined not via solving bounded system of equations, but in a way directly based on the residual of equation for the corresponding unknown at either a node or a cell.

A staggered arrangement of variables is used, this means that the pressure, density, and internal energy are located at the usual cell centres, whereas the velocity vectors are positioned at the displaced cell centres which are the vertices of usual cells.

The three-dimensional Navier-Stokes equations are solved via the Newton iteration procedure. The initial guesses are taken for the time \(t + \Delta t\) as known values for time \(t\), and the time step \(\Delta t\) is chosen with the requirement to provide the convergence within an approximately given number of iterations; then the divergence will be avoided due that restriction of time step. The introduction of artificial relations between the variations of quantities at the nearest nodes or cells and the use of approximate equality \(e' \approx -e\) relating the geometric coefficients of both displaced and usual cells, make it possible to obtain formulas for correct rates of change of the residuals of equations.
1 INTRODUCTION

The Newton procedure can diverge if the initial guesses differ significantly from the target values. If these initial guesses are taken for the time $t + \Delta t$ as the values known for the time $t$, and the time step $\Delta t$ is chosen with the requirement to provide convergence within an approximately given number of iterations, then the divergence will be avoided due to such a restriction upon the time step. We apply arbitrary polyhedral cells. The so-called staggered arrangement is used (see \textsuperscript{2}): the values of the density $\rho$, the internal energy $I$, and the pressure $p$ are assigned to the centroids of cells $j$, while the speed $\mathbf{u}$ (with components $u, v, w$) and the $x, y, z$ co-ordinates are related to the nodes $i$ which are the vertices of the polyhedral cells. On every step $\Delta t$, four (in average) global iterations are carried out. Within a global iteration the corrections of the specific internal energy of gas are determined at every cell by the values of residuals of the energy equation and the continuity equation. The density is determined from the state equation under a pressure not varying during an iteration. Next, 4 to 5 inner pressure correction iterations are carried out to correct the pressure and determine the velocity at nodes. With the help of relations between corrections of pressure and density in adiabatic approximation, these corrections are determined in cells by the value of residual of the equation of continuity. The internal energy is obtained from the state equation. The corrections of velocity afterwards are determined via the values of residuals of the equation of momentum transfer and the internal iterations are carried out further up to the fulfilment of a convergence criterion.

To use a time steps which were as large as possible, it is important to possess correct rates of the change of residuals (CRCR). We suggested\textsuperscript{1} a method for obtaining formulas of CRCR for solving discretized (finite difference) Navier-Stokes equations with the Newton iteration procedure. We discretize the Navier-Stokes equations by using a weighted scheme with the weight $\omega$. To realise the Newton-type iteration scheme and in order to avoid solving large linear systems of equations for cells $j$ or for nodes $i$, which contain the unknowns $\delta p, \delta \rho, \delta I$ not only at the cell $j$ but also at the cells $j'$ neighbouring with the cell $j$ or contain the unknowns $\delta \mathbf{u}$ not only at the node $i$ but also at the nodes $i'$ neighbouring with the node $i$, we replace the unknown relations between the variations of quantities at nearest cells $j$ and $j'$ or nodes $i$ and $i'$ by artificial ones. The introduction of artificial relations between the variations of quantities at nearest nodes or cells and the use of approximate equality $c' \approx -c$ relating geometric coefficients of both displaced and usual cells make it possible to obtain formulas for CRCR.

We replace unknown relations between the quantities at nearest nodes or cells by the artificial ones. Thus, in these formulas, the following parameters arise: $\omega_{p0}, \omega_{u0}, \omega_{I0}, \omega_{\rho u0}, \omega_{\rho uu0}$. They express the artificially given relations between the variations of quantities indicated in the subscripts (for example, $\delta \rho u_{j'} = \omega_{\rho uu0} \delta \rho u_j$). As soon as the formulas for CRCR have been deduced, one can arrange these parameters in such a way that a divergence will be prevented. For example, in our computation, we take the parameters $\omega_{p0}, \omega_{u0}, \omega_{I0}, \omega_{\rho u0}, \omega_{\rho uu0}$ equal to $-1$. This way is similar to that in \textsuperscript{3}, where we had $\omega_{p0} = -1$; in the same paper the quantity $\omega_{p0}$ was treated as the derivative of pressure in the adjacent cell $j'$ with respect.
to the pressure in the cell \( j \) under consideration. To explain the formulas of CRCR, let us consider an example in the one-dimensional case. For the inner pressure correction iteration, the following approximation is obtained for the variation of the residual of the mass conservation equation at the cell \( j \):

\[
\delta Q_{\rho j} = \delta \frac{\partial \rho}{\partial t} + \frac{1}{\Delta t} \delta \text{div}(\text{grad} \rho) = \left[ \frac{\partial \rho}{\partial p} \Delta t + (1 - \omega p_0) \omega^2 \Delta t \frac{2}{h^2} \right] \delta p_j .
\]

Earlier, in obtaining a formula of the rate of change of residual for a certain equation with the unknown \( q \), some authors had to neglect \( q \) at points adjacent to the point under consideration. To avoid the divergence, they usually took the relaxation parameter \( \omega_h = 0.5 \). This is equivalent to assigning \( \omega q_0 = 0 \) and \( \omega = 0.5 \) in our method; however, we prefer to put \( \omega q_0 = -1 \) and \( \omega = 1 \) in order to achieve more intrinsic contributions of all terms.

Generally speaking, the opposite signs of quantities' changes are not something unusual: for example, a change of velocity at a certain node may result in changes of the densities at two cells adjacent to this node. Clearly, these changes of densities are of the opposite signs. In view of the state equation, the same is valid for the pressure.

In \( \partial \frac{Q_{\rho}}{\partial p^n} \) was obtained numerically due to a small pressure change \( \delta p_0 \) introduced for all cells at the first step of iteration (see \( ^2 \), p. 144) and afterwards \( \delta Q_{\rho} \) was determined. Following our method, this corresponds to \( \omega p_0 = 1 \), so in the formula of CRCR an important term vanishes and the iteration procedure will be ineffective for some cases. Obviously, it was cumbersome to set numerically the changes of \( \delta p_0 \) that would produce distinct signs at different cells. Therefore a numerical determination of CRCR cannot be a priori effective.

We should note that our method develops the results in paper \( ^2 \). We succeeded in developing an analytic method for determination of CRCR of all the Navier-Stokes equations, with their interrelationship taken into account. Our new numerical method for solving the three-dimensional Navier-Stokes equations published previously \( ^1 \) is to be studied theoretically for the most simple case of one-dimensional acoustic equations. The convergence of the iteration scheme is proved here.

2 DIFFERENTIAL EQUATIONS

To describe a flow of a viscous heat-conducting gas in the presence of gravity, we use the Navier-Stokes equations in the Euler co-ordinates for the density \( \rho \), the velocity vector \( \mathbf{u}(u,v,w) \), and the specific internal energy \( I \) along with the state equation for the pressure \( p \):

\[
\frac{\partial \rho}{\partial t} + \text{div} \rho \mathbf{u} = 0 ,
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \text{div} \rho \mathbf{uu} = \rho \mathbf{g} - \mathbf{V} p + \text{div} \mathbf{P}_{\text{visc}} ,
\]
\[ \frac{\partial \rho I}{\partial t} + \text{div} \rho \mathbf{u} = \text{div} \left( \frac{\lambda}{c_v} \nabla I \right) + (\mathbf{P} \cdot \nabla \mathbf{u}), \]

\[ p = (\gamma_{\text{act}} - 1) \rho (I - I_{\text{noact}}(I)), \quad (1) \]

\[ \mathbf{P}_{\text{visc}} \equiv \{ \tau_{ij} \} = \left\{ -\frac{1}{3} \mu \epsilon_{kk} \delta_{ij} + \mu \epsilon_{ij} \right\}, \quad \mathbf{P} = -p \{ \delta_{ij} \} + \mathbf{P}_{\text{visc}}, \quad (2) \]

where \( g \) is the gravity acceleration. The components of the strain velocity tensor are as follows:

\[ e_{ij} = \partial u_i / \partial x_j + \partial u_j / \partial x_i. \quad (3) \]

In Eq. (1) \( \gamma_{\text{act}} = c_{\text{act}}/c_{\text{Vac}} \) means the ratio of thermal capacities for active (translational and rotational) degrees of freedom, while \( I_{\text{noact}}(I) \) is determined from the relations:

\[ c_{\text{Vac}} = \frac{1}{\gamma_{\text{act}} - 1} \cdot \frac{k}{m}; \quad I_{\text{act}} = c_{\text{Vac}} T, \quad \frac{dI_{\text{noact}}}{dT} = c_{\text{Vac}} (T), \quad I_{\text{noact}}(T = 0) = 0, \quad I = I_{\text{act}} + I_{\text{noact}}. \quad (4) \]

Here \( k \) is the Boltzmann constant, \( m \) the molecular mass of the gas, and \( T \) the absolute temperature.

### 3 BOUNDARY CONDITIONS

![Figure 1: Schematic representation of positional relationship of the actual and fictitious nodes (i) and cells (j).](image)

To assign the boundary conditions, we will use fictitious boundary cells from the outside of the solution domain. A fictitious boundary cell is said to be degenerate (possesses zero volume) if it is adjoined to a usual cell from the solid body side. All other fictitious boundary cells are said to be usual (thus possessing a nonzero volume). On Fig. 1 the subscript
\( j,\textit{fict,open} \) stands for a fictitious usual cell adjacent to an actual cell \( j \) from the side of open boundary. The subscripts \( j,\textit{fict,rig,open} \) and \( j,\textit{fict,rig} \) stand for the fictitious degenerate cells coinciding with the rigid faces of the cells \( j,\textit{fict,open} \) and \( j \), respectively. The subscripts \( i \) and \( i,\textit{rig} \) are related to the nodes inside the computation domain and on its wall (on a rigid surface), respectively. The subscripts \( i,\textit{fict} \) and \( i,\textit{fict,rig} \) correspond to respective nodes on the open boundary. All the above cells and nodes may possess the corresponding symmetric cells and nodes, which are not shown on Fig. 1.

On the open boundaries, in the boundary cells \( j,\textit{fict,open} \) the quantities either \( p, \rho, I \) or \( \rho, I \) must be given. In case of \( p, \rho, I \) being given (this, as a rule, is the outlet), the velocity \( u \) at the boundary nodes \( i,\textit{fict} \) and \( i,\textit{fict,rig} \) will be defined by assigning their values at the internal nodes \( i \) and \( i,\textit{rig} \), where the velocities are obtained via calculation. This is necessary in order to calculate the strain velocity tensors in the boundary cells \( j,\textit{fict,open} \). These tensors are then applied to calculate the viscous stress tensors' divergence at the nodes \( i \) for determination of the velocity at such a node. In the case where only \( \rho, I \) are given in the cells \( j,\textit{fict,open} \) (as a rule, this is valid for the inlet), the velocities must be a priori given at the nodes \( i,\textit{fict} \) and \( i,\textit{fict,rig} \), and at the adjacent nodes \( i \) and \( i,\textit{rig} \). Indeed, at the nodes \( i,\textit{fict} \) and \( i,\textit{fict,rig} \) we need not to know the value of velocity; however, we do this because in the program, the strain velocity tensors are calculated at all boundary cells \( j,\textit{fict,open} \). In the case of the outlet, the internal energy \( I \) and density \( \rho \) in the boundary cells \( j,\textit{fict,open} \) are necessary for calculation of the internal energy gradient \( \nabla I_i \) and the momentum \( \rho_i u_i \), respectively, at the internal nodes \( i \) nearest to open boundaries. In the case of the inlet, the internal energy \( I \) in the boundary cells \( j,\textit{fict,open} \) is necessary for calculation of the internal energy gradient \( \nabla I_i \) at the internal nodes \( i \) nearest to open boundaries. What is more, in the case of the inlet, the internal energy \( I \) and density \( \rho \) in the boundary cells \( j,\textit{fict,open} \) are necessary for calculation of the internal energy flows and the mass flows inside the domain. The same may be necessary in the case of the outlet as well.

Thus, as we noted earlier, in spite of the necessity to know thermodynamic values and velocity not in all boundary nodes and cells, for the sake of computation convenience these are determined and assigned everywhere.

The open boundaries are assumed to be sufficiently distant from domains possessing high gradients.

To calculate the parameters of a gas moving in open devices, we use the continuity condition of the flow near the open boundary (see \(^3\)) and in presence of the gravity. Therefore the boundary conditions

\[
\begin{align*}
  p_{j,\textit{fict,open}} &= (1 - \Delta t/\tau) p_j e^{x_j} \rho_j \left( r_{j,\textit{fict,open}} - r_{j} \right) + \left( \Delta t/\tau \right) p_\infty e^{x_j} \rho_\infty \left( r_{j,\textit{fict,open}} - r_\infty \right) / p_\infty, \\
  I_{j,\textit{fict,open}} &= (1 - \Delta t/\tau) I_j + \left( \Delta t/\tau \right) I_\infty
\end{align*}
\]

have been taken into account. The value \( \rho_{j,\textit{fict,open}} \) is determined via \( p_{j,\textit{fict,open}} \) and \( I_{j,\textit{fict,open}} \) through the state equation. The values \( \rho_\infty \) and \( p_\infty \) are the density and pressure, respectively, at infinity point for a fixed height which is defined by a position vector \( r_\infty \). For a viscous steady
flow in a tube, the spatial pressure distribution for $\Delta t/\tau < 1$ is same as for $\Delta t/\tau = 1$ if the tube length has been extended by $(\tau / \Delta t)h$ in the output direction. The relaxation parameter $\Delta t/\tau$ is taken equal to 0.01.

We should note that it is more correct if, at the outlet, in the boundary cells $j_{fict,open}$ we calculate the value of density by solving by means of iteration technique the finite-difference equation of continuity, the value of pressure by the above formula, and the internal energy via $p_{j_{fict,open}}$ and $\rho_{j_{fict,open}}$ through the state equation. This makes it possible, in using the double accuracy for all values (REAL(8)), to achieve the equality between mass flows on both inlet and outlet for a stabilised current with the accuracy $10^{-10}$ for given relative errors (see in what follows) $\varepsilon_{\rho,I} = 0.2 \cdot 10^{-10}$, $\varepsilon_u = 0.3 \cdot 10^{-10}$, $\varepsilon_{u(P-link)} = 0.2 \cdot 10^{-10}$ and the step $\Delta t = h/u_{flow}$. The reduction of the value $\varepsilon_{\rho,I}$, $\varepsilon_u$, $\varepsilon_{u(P-link)}$ by $10^4$ times leads to a reduction of the step $\Delta t$ by almost 100 times; however, in this situation, the mass balance is preserved with the restrictedly small (for the chosen double accuracy) error of $10^{-14}$.

In contrast to\(^1\), $\nabla I_{i,rig}$ at the nodes $i,rig$ lying on a solid surface are calculated by averaging the vectors $\nabla I_j$ in the cells $j$ near the solid surface. $\nabla I_j$ is calculated via the given values $I_{i,rig}$. In\(^1\), $\nabla I_{i,rig}$ at the nodes $i,rig$ lying on a solid surface were calculated by means of the Newton-type iteration scheme so that $\nabla I_j$ (defined from $\nabla I_{i,rig}$) in the cells $j$ near the solid surface was equal to $\nabla I_j$ calculated via the given values $I_{i,rig}$. This iteration process turned to be divergent; however, it was not leading to an essential error while in the capacity of initial approximations we took averaged values from cells near a solid node and limited the number of iterations (in fact, we did not leave far such an initial approximation which now is used in the capacity of a final value). As soon as we started to take as initial approximations the values from the previous time layer $t$, the error turned to be evident.

At rigid walls, for $\mu \neq 0$, we put $u = 0$.

4 INITIAL CONDITIONS

The problem of the start of computation deserves a certain attention. At the input we give a parabolic distribution of velocity in accordance with Poiseuille law for incompressible viscous fully developed pipe flow. The value of velocity is determined by the input volume flow $Q_{inp}$. If we start the computation from the initial immobile gas state, assigning straight away the large value of input volume flow on the boundary, then the initial step $\Delta t$ is automatically set up small with a value of order $h/a$ (here $a$ is the sound speed). The computation process takes a very long time because it then corresponds to a real stabilising process of wave transmission. If this process is not of our interest, then it turns out that, if one assigns the input volume flow assumed to change by a linear law with respect to time from zero value to a given one during a time interval $t_{relax}$ approximately equalling $20\Delta t_{max}$, then the step grows quickly from the initial order of $h/a$ to $\Delta t_{max}$, and the process stabilises within 1000 to 2000 time steps.
5 NODES, FACES AND CELLS, FINITE DIFFERENCE APPROXIMATION OF
DIFFERENTIAL OPERATORS AND OTHER TERMS

In this section we briefly describe formulas for geometric coefficients and finite difference
approximations of spatial operators, which were obtained in\(^1\).

5.1 Nodes, faces and cells

The faces and geometric coefficient \(c^l\) at a point \(l\) are constructed in the following way. We define the face \(m\) as a surface passing through some given edges. The geometric
coefficient \(c^m\) is set to be equal to the surface normal vector directed outside from the cell:

\[
c^m = \int_{S_m} d\sigma.
\]

Draw a plane perpendicular to \(c^m\). Next, drop perpendiculars onto this plane from the
vertices \(l\) of the face \(m\). Next, for the resulting plane polygon we find the centroid (centre of
gravity) \(O\).

![Diagram of the projection of the face](image)

Figure 2: The projection of the face \(m\) is a plane polygon.

The polygon is divided into a set of quadrangles (see on Fig. 2). The ratio of the square of the
quadrangle \(L_1L_2O\) (\(L_1\) and \(L_2\) are the middles of polygon's edges) to the square of the
polygon gives us the quantity \(q^{ml}\).

\[
q^{ml} = \frac{S_{L_1L_2O}}{c^m}, \quad \sum l q^{ml} = 1.
\]

The face \(m\) can be considered as a set of triangles \(mnl\) with a point \(m\) defined as
\[ \mathbf{r}_m = \sum_{l=1}^{N_m} q^{ml} \mathbf{r}_l . \]  

(5)

Here \( N_m \) stays for the number of vertices of the face \( m \). In other words, \( S_m \) is a surface obtained by rotation of a straight-line segment around the point \( m \) with the end of segment running along the straight edges. For the sake of simplicity, here and in some further places we will omit the limits of sums.

The face \( S_m \) has the properties:

\[ \mathbf{r}_{mO} = \mathbf{r}_m - \mathbf{r}_O \parallel \sigma^m, \]

the quantity \( q^{ml} \) is determined only by the points \( l \); the point \( \mathbf{r}_m \) of the face \( m \) is determined only by boundary straight edges and the result of (5) does not depend on the number \( N_m \) of the point \( l \). In other words, by inserting additional vertices into the boundary straight edges we do not change \( \mathbf{r}_m \) and therefore the face \( m \) as well.

The following property of the face \( S_m \) is also of interest. Let \( S_{m\perp} \) be the projection of \( S_m \) onto the plane that passes through \( m \) and is perpendicular to \( \sigma^m \). The volumes between \( S_m \) and \( S_{m\perp} \) on the opposite sides of \( S_{m\perp} \) are equal to each other.

5.2 Finite difference approximation

Here we give the formulas\(^1\) for finite-difference approximation of differential operators and for determination of quantities in a cell provided that the quantities are known at the cell vertices. We also give an estimate of approximation inaccuracy for various faces, cells, and geometric coefficients.

The geometric coefficient \( c^{ml} \) of the face \( m \) at the point \( l \) is introduced as follows

\[ c^{ml} = \frac{c^m q^{ml} + 2 \sigma_{l_1l_2m}}{3}. \]

(6)

Here \( l_1 \) and \( l_2 \) are the middles of the edges \( nl \) and \( lk \), respectively, \( \sigma_{l_1l_2m} \) is the surface normal vector of the quadrangle \( l_1l_2m \).

For the general case of a non-planar face, we have

\[ \int_{S_m} \mathbf{r} \cdot d\sigma = \sum_l \mathbf{r}_l \cdot c^{ml} = \mathbf{r}_m \cdot c^m = \sum_l \mathbf{r}_l \cdot q^{ml} c^m = \sum_l \mathbf{r}_l \cdot \sigma_{l_1l_2m}. \]

Clearly,

\[ \int_{S_m} d\sigma = c^m = \sum_l c^{ml} = \sum_l q^{ml} c^m = \sum_l \sigma_{l_1l_2m}. \]
Next, for the surface $S$ of a cell with the number of faces $N_f$, we have

$$\int_S d\sigma = \sum_{m=1}^{N_f} c^m = \sum_{m=1}^{N_f} \sum_{l=1}^{N_m} c^{ml} = \sum_{m=1}^{N_f} \sum_{l=1}^{N_m} q^{ml} c^m = \sum_{m=1}^{N_f} \sum_{l=1}^{N_m} \sigma_{l||z,m} = 0.$$ 

In the case of a planar cell face, we have

$$c^{ml} = c^m q^{ml} = \sigma_{l||z,m}.$$ 

For the general case of a non-planar face, these vectors differ by both their magnitude and direction. The relative difference may be characterised by the quantity $\Delta_{\text{face}}$, which characterises also the non-flatness of the face

$$\Delta_{\text{face}} = \max_l \left| \frac{r_{lm} \cdot c^m}{r_{lm} c^m} \right|.$$ 

Let us denote by $c^l$ the geometric coefficient at vertex $l$ of the cell; $c^l$ consists of components $c^{ml}$ related to every face $m$ which passes through the vertex $l$

$$c^l = \sum_m c^{ml}. \quad (7)$$

For hexahedrons with planar faces it can be shown that the expression for $c^l$ coincides with the formula suggested by D. C. Barnes in $^5$. Coefficient $c^l$ has a clear geometric meaning. In case of a cell with planar faces, it is the sum of the three vectors which are normal to the respective faces and possess lengths equal to the areas of quadrangles. Any quadrangle is a part of the respective face and has the four vertices: the vertex $l$ of the cell, the two centres (middles) of edges, and the face's centroid. Three of these quadrangles for the coefficient $c^4$ are shown on Fig. 3 as hatched.

![Figure 3: Geometric interpretation of the coefficient $c^4$](image)

By using the above-mentioned geometric coefficients, we may obtain the finite-difference form of quantities:
\[ V = \sum_{i=1}^{N} x_i c_i^l = \sum_{i=1}^{N} y_i c_i^l = \sum_{i=1}^{N} z_i c_i^l = \frac{1}{3} \sum_{i=1}^{N} r_i \cdot c_i^l ; \]  

(8)

Here \( N \) stands for the number of cell vertices and

\[ \sum_{i=1}^{N} y_i c_i^l = \sum_{i=1}^{N} z_i c_i^l = \ldots = \sum_{i=1}^{N} y_i c_i^l = \sum_{i=1}^{N} c_i^l = \sum_{i=1}^{N} c_i^l = \sum_{i=1}^{N} c_i^l = 0. \]  

(9)

We also will need the following formula

\[ \int_{S} r d\sigma = \sum_{i=1}^{N} r_i c_i^l , \]

which along with (8) and (9) gives us

\[ \frac{1}{V} \sum_{i=1}^{N} r_i c_i^l = \frac{1}{V} \sum_{i=1}^{N} c_i^l r_i = E , \]

where \( E \) is the unit tensor. The centre of gravity is obtained as follows

\[ r_M = \frac{1}{4V} \sum_{m} \sum_{l} c_{m} c_{l} r_{l} . \]

By using the multivariable Taylor expansion, we obtain (see 1)

\[ \nabla \Phi_M = \frac{1}{V} \sum_{m} \sum_{l} \Phi c_{m} c_{l} + O(h^2) + \]

\[ + \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial^2 \Phi}{\partial x_i \partial x_j} \frac{1}{V} \sum_{m} \int_{S} \left( x_i - x_{m i} \right) \left( x_j - x_{m j} \right) d\sigma - \sum_{l} \left( x_i - x_{m i} \right) \left( x_j - x_{m j} \right) c_{m} c_{l} \]  

(10)

The last term in (10) vanishes for a cell generated by pairs of parallel faces. This is evident since, for the corresponding opposite faces, by their absolute value the vectors \( d\sigma \) or \( c_{m} c_{l} \) are equal to each other but are oppositely directed, while the remaining multipliers coincide. To the cells with pairwise parallel faces we assign the parameter \( \Delta_{cell} = 0 \), while \( \Delta_{cell} = 1 \) for all other cells. Thus, by substituting (7) into (10), we can rewrite (10) as follows

\[ \nabla \Phi_M = \frac{1}{V} \sum_{l} \Phi c_{l} + \Delta_{cell} O(h) + O(h^2) . \]  

(11)

From (11) it directly follows that

\[ \text{div} \Phi_M = \frac{1}{V} \sum_{l} \Phi c_{l} + \Delta_{cell} O(h) + O(h^2) . \]
Thus, we can see that the central difference scheme (CDS) can supply a first order truncation error in $h$ if $\Delta_{cell} = 1$. The truncation error of the second order in $h$ is equal to zero if $\Phi$ depends on the space co-ordinates in the quadratic form; however, a first-order error in $h$ remains if $\Delta_{cell} = 1$. If the dependence of $\Phi$ on the space co-ordinates is linear, then the error vanishes for any $\Delta_{cell}$.

In the divergence’s determination the inaccuracy of the upwind difference scheme (UDS) will be of the first order in $h$ and of the first order in $\Delta_{mesh}$, here $\Delta_{mesh}$ characterises the non-uniformity of mesh spacing, i.e., the difference between the adjacent cells $j$ and $j'$

$$\Delta_{mesh} \approx \frac{h_j'}{h_j} - 1.$$  

If we introduce $\Delta_{UDS} = 1$ in case of UDS scheme being used and $\Delta_{UDS} = 0$ in case of CDS scheme, then we have

$$\text{div}\Phi_M = \frac{1}{V} \sum_l \Phi_l \cdot c^l + (\Delta_{mesh} + O(h))\Delta_{UDS} + \Delta_{cell}O(h) + O(h^2).$$

For example, the convective flux of energy is obtained as follows

$$\text{div}\rho\mathbf{u}_j = \frac{1}{V} \left\{ \sum_{m,l} \left[ (\rho l)_m \cdot \mathbf{c}^l \right] \mathbf{u}_l \cdot \mathbf{c}^m + \rho l_j \sum_{m,l} (\mathbf{u}_l - \mathbf{u}_j) \cdot \mathbf{c}^m \right\},$$

where the prime means an approximation. We take the quantity $\rho l_j$ if $\mathbf{u}_l \cdot \mathbf{c}^m \geq 0$ and the corresponding quantity from the other side of the face $m$ otherwise. Here $l$ stands for the vertex of the cell $j$. We also use the fact that $\sum_{m,l} \mathbf{c}^m = 0$.

For a more accurate calculation, the quantities $V$ and $\mathbf{r}_M$ will be determined from the formulas

$$V = \frac{1}{3} \sum_{i=1}^N (x_i - x_1) c^i_j = \frac{1}{3} \sum_{i=1}^N (y_i - y_1) c^i_j = \frac{1}{3} \sum_{i=1}^N (z_i - z_1) c^i_j \quad \text{or} \quad V = \frac{1}{3} \sum_{i=1}^N (\mathbf{r}_i - \mathbf{r}_1) \cdot \mathbf{c}^i,$$

and

$$\mathbf{r}_M = \mathbf{r}_1 + \frac{1}{4V} \sum_m (\mathbf{r}_m - \mathbf{r}_1) \cdot \sum_l \mathbf{c}^m (\mathbf{r}_l - \mathbf{r}_1).$$  \hspace{1cm} (12)$$

If we will use $q^m c^m$ instead of $c^m$, the corresponding geometric coefficient $c^i_0$,  

$$c^i_0 = \sum_m q^m c^m,$$

will appear instead of $c^i$. After a simplification, the formulas can be expressed as follows:
\[ V = \frac{1}{3} \sum_{l=1}^{N} (\mathbf{r}_l - \mathbf{r}_i) \cdot \mathbf{c}_l^i, \]  

(13)

\[ \mathbf{r}_M = \mathbf{r}_i + \frac{1}{4V} \sum_{l=1}^{N} (\mathbf{r}_l - \mathbf{r}_i) [(\mathbf{r}_l - \mathbf{r}_i) \cdot \mathbf{c}_l^i] + \Delta_{face} \mathbf{O}(h), \quad |\mathbf{O}(h)| \approx h, \]  

(14)

\[ \Phi_M = \frac{1}{3V} \sum_{l=1}^{N} [(\mathbf{r}_l - \mathbf{r}_M) \cdot \mathbf{c}_l^i] \Phi_i + \Delta_{\text{face}} \nabla \Phi_M \cdot \mathbf{O}(h) + O(h^2), \quad |\mathbf{O}(h)| \approx h, \]  

(15)

\[ \nabla \Phi_M = \frac{1 + \Delta_{\text{face}} O(1)}{V} \sum_i \Phi_i \mathbf{c}_0^i + \Delta_{\text{cell}} \mathbf{O}(h) + O(h^2), \quad |\mathbf{O}(h)| \approx h \sum_{i=1}^{3} \sum_{j=1}^{3} \left| \frac{\partial^2 \Phi}{\partial x_i \partial x_j} \right|, \]

\[ \text{div} \Phi_M = \frac{1 + \Delta_{\text{face}} O(1)}{V} \sum_i \Phi_i \cdot \mathbf{c}_0^i + \Delta_{\text{cell}} \mathbf{O}(h) + O(h^2), \quad |\mathbf{O}(h)| \approx h \sum_{i=1}^{3} \sum_{j=1}^{3} \left| \frac{\partial^2 \Phi}{\partial x_i \partial x_j} \right|. \]

In Eq. (15) the vector \( \mathbf{r}_M \) is taken from (14) as approximately determined. One can see that some additional inaccuracies appear in the formulas (with except for Eq. (13)). These formulas do not calculate and memorise \( \mathbf{r}_m \) and vectors \( \mathbf{c}_{ml} \); they deal only with the scalars \( q_{ml} \) and vectors \( \mathbf{c}_m \); therefore, they save the memory. They can be used for residuals’ computation if \( \Delta_{\text{face}} \ll 1 \); however, the geometric coefficients \( \mathbf{c}_0^i \) can always be used to compute CRFR.

5.3 Displaced cells, finite difference approximation

The above formulas make it possible to write the Navier-Stokes equations in a finite difference form. Some terms in the finite-difference equations can be obtained with the use of the above cell. Other terms use displaced cells which are constructed around the nodes. The vertices of the displaced cell are the centroids of the usual cells surrounding the node. For such displaced cells, their coefficients \( \mathbf{c}^l \) are defined in Eqs. (6), (7); however, for the new cells the position vectors \( \mathbf{r}_l \) are the centroids of usual cells. We find the approximate correlation \( \mathbf{c}^l \approx - \mathbf{c} \) between the corresponding geometric coefficient \( \mathbf{c}^l \) of displaced cell and the coefficient \( \mathbf{c} \) of the usual cell. This correlation was used in the determination of CRFR.

For correct computation we need to know the difference between a node \( i \) and the centroid (centre of gravity) \( M \) of a displaced cell around the node \( i \). The relative difference can be characterised by the following quantity:

\[ \Delta_{\text{displace}} = \frac{|\mathbf{r}_i - \mathbf{r}_M|}{h}. \]
This quantity is close to \( \Delta_{\text{mesh}} \). If we do not use Eq. (12) for displaced cell and instead of \( r_M \) the position vector \( r_i \) of node \( i \) will be taken, then an additional inaccuracy term \( \Delta_{\text{displace}} O(h) \) appears in the corresponding formulas. For example, Eq. (11) gives us

\[
\nabla \Phi_i = \frac{1}{V} \sum_l \Phi_l c' + \left( \Delta_{\text{cell}} + \Delta_{\text{displace}} \right) \mathcal{O}(h) + \mathcal{O}(h^2).
\]

6 FINITE-DIFFERENCE EQUATIONS

If all the necessary quantities for the time \( t' = t \) are known, then to determine the unknown quantities for \( t^{n+1} = t + \Delta t \) we use the discretized Navier-Stokes equations with a weighted scheme with the weight \( \omega \)

\[
\begin{align*}
\frac{Q_\rho}{\Delta t} &= \frac{1}{\Delta t} \left( \rho^{n+1} - \rho^n \right) + \omega \, \text{div} \rho^{n+1} \mathbf{u}^{n+1} + (1 - \omega) \, \text{div} \rho^n \mathbf{u}^n, \quad Q_\rho = 0. \\
\frac{Q_\alpha}{\Delta t} &= \frac{1}{\Delta t} \left( \rho^{n+1} \mathbf{u}^{n+1} - \rho^n \mathbf{u}^n \right) - \left[ \omega \, \rho^{n+1} + (1 - \omega) \, \rho^n \right] \mathbf{g} + \left[ \omega \nabla p^{n+1} + (1 - \omega) \nabla p^n \right] - \\
&- \omega \text{div} \mathbf{P}^{n+1} - (1 - \omega) \text{div} \mathbf{P}^n + \omega \text{div} \rho^{n+1} \mathbf{u}^{n+1} \mathbf{u}^{n+1} + (1 - \omega) \text{div} \rho^n \mathbf{u}^n \mathbf{u}^n, \quad Q_\alpha = 0. \\
\frac{Q_i}{\Delta t} &= \frac{1}{\Delta t} \left( \rho^{n+1} I^{n+1} - \rho^n I^n \right) - \omega \mathbf{P}^{n+1} \cdot \nabla \mathbf{u}^{n+1} - (1 - \omega) \mathbf{P}^n \cdot \nabla \mathbf{u}^n - \omega \text{div} \left( \frac{\alpha^{n+1}}{c_V^n} \nabla I^{n+1} \right) - \\
&- (1 - \omega) \text{div} \left( \frac{\alpha^n}{c_V^n} \nabla I^n \right) + \omega \text{div} \left( \rho^{n+1} I^{n+1} \mathbf{u}^{n+1} \right) + (1 - \omega) \text{div} \left( \rho^n I^n \mathbf{u}^n \right), \quad Q_i = 0.
\end{align*}
\]

To calculate the spatial differential operators and other terms we use the formulas given in the previous section.

7 CORRECT RATES OF THE CHANGE OF RESIDUALS

For the initial guesses at the time \( t' = t \) we take the values at the time \( t \). On every global iteration step \( L \) for the known quantities \( \rho_{j,J}^{n+1}, \mathbf{P}_{j,J}^{n+1}, I_{j,J}^{n+1} \) and \( \mathbf{u}_{j,i}^{n+1} \) in all cells \( j \) and nodes \( i \) for the time \( t + \Delta t \) we determine the residuals \( Q_\rho, Q_\alpha, Q_i \) in every cell \( j \) and the residuals \( Q_\alpha, Q_i \) in every node \( i \). To realise the Newton-type iteration scheme and in order to avoid solving large linear systems of equations for cells \( j \) and for nodes \( i \), let us express the variations of residuals at the iteration \( L \) as follows

\[
\begin{align*}
\delta Q_{\rho, j} &= \frac{\partial Q_{\rho}}{\partial \rho} \delta \rho_{j,J}^{n+1} + \frac{\partial Q_{\rho}}{\partial I} \delta I_{j,J}^{n+1}, \quad \delta Q_{\alpha, j} = \frac{\partial Q_{\alpha}}{\partial \rho} \delta \rho_{j,J}^{n+1} + \frac{\partial Q_{\alpha}}{\partial I} \delta I_{j,J}^{n+1}. \\
\delta Q_{i, j} &= A_{j} \delta \mathbf{u}_{j,i}^{n+1}, \quad \delta Q_{i, j} = A_{j} \delta \mathbf{u}_{j,i}^{n+1}.
\end{align*}
\]
The variations of the residuals at the inner iteration \( L_p \) can be expressed as follows

\[
\delta Q_{p,j} \approx \frac{\partial Q_p}{\partial p} \delta p_{j,L+1,L,p}^{n+1},
\]

\[
\delta Q_{u,i} \approx A_{u,j} \delta u_{i,L+1,L,p}^{n+1}.
\]

Let us write here the expressions revealing CRCR and derived earlier in\(^1\):

\[
\delta Q_{p,j} = \left[ \frac{1}{\Delta t} + B_1 \right] \delta p_{j,L+1,L,p}^{n+1} + B_2 \delta p_{j}^{n+1},
\]

\[
\delta Q_{i,j} = \left[ \frac{I_{i}^{n+1}}{\Delta t} + B_i C_3 \right] \delta p_{j,L+1,L,p}^{n+1} + \left[ \frac{I_{j}^{n+1}}{\Delta t} + B_j C_3 + \omega(1 - \omega_t)C_i \left( \frac{\rho_j}{C_y} \right)^{n+1} \right] \delta I_{j,L+1}^{n+1}.
\]

To reduce the calculation, we determine \( A_i \) by means of the process of averaging in the volume of a displaced cell \( i \) by means of \( A_j \). Next, \( A_j \) is obtained via the formula

\[
A_j = \frac{1}{\Delta t} \rho_j^{n+1} + \omega^2 \Delta t \frac{1 - \omega_t}{3} C_1 \gamma(I_j^{n+1})p_j^{n+1} + \omega \frac{7\mu(1 - \omega_t)}{9} C_1.
\]

The following expressions are for the inner pressure correction iteration:

\[
\delta Q_{p,j} \approx \left[ \frac{1}{\Delta t} + B_1 C_4 \right] \frac{1}{C_4} \delta p_{j,L+1,L,p}^{n+1}, \quad A_p = \rho_p^{n+1} \left( \frac{1}{\Delta t} + \frac{\omega \omega_t \mu_{elt}}{h_b} \right).
\]

The coefficients in the above expressions are

\[
C_1 = \frac{1}{V_j} \sum_i (e_i^j)^2, \quad e_i = \sum_m e_{m,i}, \quad C_2 = (1 - \omega_t) \rho_j^{n+1} + (1 - \omega_{\rho\omega}) \frac{(u_j^{n+1})^2}{3},
\]

\[
C_3 = I_j^{n+1} + \frac{p_j^{n+1}}{\rho_j^{n+1}}, \quad C_4 = \gamma(1 + 1) \frac{p_j^{n+1}}{\rho_j^{n+1}}, \quad h_b = V_j / \sum_m |\rho_j^{n+1}|,
\]

\[
B_1 = \omega^2 \Delta t C_1 C_2, \quad B_2 = \omega^2 \Delta t (1 - \omega_t) \left( \gamma(I_j^{n+1}) - 1 \right) \rho_j^{n+1} C_1, \quad B_3 = (1 - \omega_t) \omega^2 \Delta t C_1.
\]

In our computation we took \( \omega_{ap} = 0.2 \). The above terms are obtained via the initial iteration guesses, i.e., in fact, via the values assigned for the time \( t \).

8 SEQUENCE OF ITERATION CYCLES

We\(^1\) determine increments \( \delta I_{j,L}^{n+1} \) in the Newton global iteration \( L \) as follows
\[ \delta I_{L}^{n+1} = - \frac{Q_{p}^{n+1} \left( I_{L}^{n+1}, p_{L}^{n+1}, \mathbf{u}_{L}^{n+1} \right) \partial Q_{p} / \partial \rho_{L}^{n+1} - Q_{J} \left( \rho_{Lj}^{n+1}, I_{Lj}^{n+1}, p_{Lj}^{n+1}, \mathbf{u}_{Lj}^{n+1} \right) \partial Q_{J} / \partial \rho_{Lj}^{n+1} }{Q_{p}}. \]

One can easily verify that the discriminant \( D_{Q} \)

\[ D_{Q} = \frac{\partial Q_{p}}{\partial \rho} \frac{\partial Q_{J}}{\partial I} - \frac{\partial Q_{J}}{\partial \rho} \frac{\partial Q_{p}}{\partial I} \]

always exceeds zero. Then we have

\[ I_{j,L+1}^{n+1} = I_{j,L+1}^{n+1} + \omega_{j} \delta I_{j,L}^{n+1}. \]

Here to the relaxation parameter \( \omega_{L} \) (which is \( \omega_{I} \) for energy) we assigned the value 1. By determining \( \rho_{j,L+1}^{n+1} \) from the state equation via \( I_{j,L+1}^{n+1} \) and \( p_{j,L+1}^{n+1} = p_{j,L}^{n+1} \), we find \( \mathbf{u}_{j,L+1}^{n+1} \) via the equations

\[ A_{L} \delta \mathbf{u}_{L}^{n+1} = -Q_{a} \left( \rho_{L}^{n+1}, I_{L}^{n+1}, p_{L}^{n+1}, \mathbf{u}_{L}^{n+1} \right), \]

\[ \mathbf{u}_{L}^{n+1} = \mathbf{u}_{L}^{n+1} + \delta \mathbf{u}_{L}^{n+1}. \]

Now we pass to the introduction of the pressure correction procedure into the inner iterations. In the inner iteration \( L_{p} \) the corrected values of pressure are determined from the following equations

\[ \delta p_{L}^{n+1} = \frac{Q_{p} \left( \rho_{L}^{n+1}, I_{L}^{n+1}, p_{L}^{n+1}, \mathbf{u}_{L}^{n+1} \right) \partial Q_{p} / \partial p_{L}}{\partial Q_{p} / \partial \rho}, \]

\[ p_{L}^{n+1} = p_{L}^{n+1} + \omega_{p} \delta p_{L}^{n+1}. \]

Here \( \rho_{L}^{n+1}, I_{L}^{n+1}, \mathbf{u}_{L}^{n+1} \) expresses the state equation and is used only for computation of the term \( \partial \rho / \partial t = (\rho^{n+1} - \rho^{n}) / \Delta t \) (in our computation the relaxation parameter \( \omega_{p} \) was assumed to be equal to 1). Afterwards we determine \( \mathbf{u}_{L}^{n+1} \) via the equations

\[ A_{p} \delta \mathbf{u}_{L}^{n+1} = -Q_{a} \left( \rho_{L}^{n+1}, I_{L}^{n+1}, p_{L}^{n+1}, \mathbf{u}_{L}^{n+1} \right), \]

\[ \mathbf{u}_{L}^{n+1} = \mathbf{u}_{L}^{n+1} + \delta \mathbf{u}_{L}^{n+1}. \]

Further, let us describe the proper sequence of iterations. We start both the global and inner iterations with \( L=0, L_{p}=0 \). We restrict the inner iteration \( L_{p} \) by the limits for \( L_{p} +1 \) from 2 to 5. If the \( L_{p} +1 \geq 2 \) and

\[ \delta u_{(p-link)} = \max \left( \| \delta u \| + \| \delta v \| + \| \delta v \| \right) < e_{u(p-link)}, \]

or \( L_{p} +1 = 5 \), then we stop the inner iteration \( L_{p} \). Otherwise we move to the next iteration \( L_{p} +1 \). After stopping the inner pressure correction iterations we change the density and internal
energy by means of adiabatic approximation so that new values of them correspond to the new value of pressure with the state equation. Then we go to the next global iteration \( L^{+1} \).

We restrict the global iteration \( L \) by the limits from 2 to 15 for \( L^{+1} \) if the \( L^{+1} \geq 2 \) and

\[
\delta_{\rho,1} = \max |\delta \rho|/\rho_{\max} + \max |\delta l|/l_{\max} < \varepsilon_{\rho,1}, \tag{16}
\]

\[
\delta_\alpha = \max (|\delta u| + |\delta v| + |\delta w|)/u_{\max} < \varepsilon_\alpha, \tag{17}
\]

and for the last inner iteration of preceding global iteration we have

\[
\delta_{\alpha(p-link)} = \max (|\delta u| + |\delta v| + |\delta w|)/u_{\max} < \varepsilon_{\alpha(p-link)}, \tag{18}
\]

or \( L^{+1}=15 \), then we stop the global iteration \( L \). Otherwise we go to the first \( L_0 = 0 \) inner iteration. After a catastrophic stop of the global iterations (if \( L^{+1}=15 \)) we sharply decrease the time step \( \Delta t_{\text{new}} = 0.75 \Delta t_{\text{old}} \) and begin the iteration process again with the same \( t \). After a regular stop of the global iterations (i.e., if \( L^{+1} < 15 \)) in accordance with the convergence criteria (16)-(18), we pass to the next time \( t + \Delta t_{\text{new}} \) and change the time step in accordance with the sum of the three last numbers of the preceding global iterations, i.e., \( \Delta t_{\text{new}} = 0.9 \Delta t_{\text{old}} \) if the sum exceeds 13, \( \Delta t_{\text{new}} = 1.01 \Delta t_{\text{old}} \) if the sum is lesser than 10. The previous choice establishes the number of global iterations equal to 4 on average as well as the corresponding value of the time step.

The above-stated iteration scheme is not unique; successful calculations were also executed by means various modifications of the scheme. For example, one can take into account the change of \( \rho \) in the term \( \text{div} \rho^{n+1}u^{n+1} \) in the continuity equation for inner pressure correction iterations. One can either recalculate or leave recalculation of the term \( \text{div} P_{\text{visc},i} \) during the inner pressure correction iterations. In the global iterations one can omit the determination of velocity. Successful computations were carried out with modified values of CRCR.

9 NUMERICAL TESTING OF THE METHOD

We present some results on modelling for a heated viscous gas flow (Argon) in a tube of an electrothermal vapourisation (ETV) system. This problem was used for both testing and deriving of an effective numerical method. It also helped us to formulate the final version of the formulas of CRCR in the Newton global iteration procedure and the Newton inner pressure correction iteration procedure. The chosen values of tube length and the regime of heating only simulate a real process. To reduce the calculation we consider the axial symmetry case; however, since the program is designed for a 3D calculation, the 3D cells are constructed. Let us note that the region of tube is not filled completely. The scalar quantities in symmetric cells and nodes are taken from the ordinary cells and nodes, and the vector quantities are defined from the ordinary nodes by rotating around the symmetry axis. In Fig. 7 illustrates the scheme of the tube and faces of cells in longitudinal and radial planes.

The wall temperature \( T_w(x,t) \) in ETV depends on both the longitudinal co-ordinate \( x \) and the time \( t \). The temperature dependence \( T_w(0,t) \) at the tube’s centre was taken (with rejection
of a part of the interval with constant temperature) from\textsuperscript{6} and it is shown in Fig. 4. It increases from $T_0=300K$ to 450K within the time $t$ passing from 2s to 3s; afterwards it rises from 450K to 2750K for the time $t$ changing from 4s to 5s, then it decreases from 2750K to $T_0$ for the time $t$ increasing from 6s to 17s. The following spatial dependence of the wall temperature is given for $x$ in mm

\[
\text{for } |x| > 16.8 \quad T_w(x, t) = T_0 = 300K,
\]

\[
\text{for } 14 \leq |x| \leq 16.8 \quad T_w(x, t) = \frac{16.8 - |x|}{2.8} \max[T_0, T_w(0, t)/2] + \frac{|x| - 14}{2.8} T_0,
\]

which constitutes a linear interpolation.

\[
\text{for } |x| \leq 14 \quad T_w(x, t) = \max[T_0, T_w(0, t)\left(1/4|x|^{2}\right)].
\]

This equation contains the Gaussian distribution described in\textsuperscript{7} as the closest fitting to the experimental dependence.

To determine the change in volume with respect to the time, in\textsuperscript{6} a simplistic model was suggested which includes: 1) the gas temperature inherits the wall temperature at any given time $t$ and position $x$ in the system, and 2) the pressure in the system is assumed to be constant. In a similar way, we obtain an analytic formula for the mass flow balance. Let $x_a$ and $x_b$ be the co-ordinates of tube ends, the output and input volume flow through the ends be equal to $Q_a$ and $Q_b=Q_{inp}$, respectively, the output and input mass flow through the ends be $m_a = \rho_a Q_a$ and $m_b = \rho_b Q_{inp}$, respectively. Assume that the cross-section area is $A(x)$ and the mass
of gas in the region \([x_a, x_b]\) is \(M\). For the input flow we have \(\rho_0=\rho_b\) which is the density at \(T_0=300\text{K}\). Therefore

\[
M = \int_{x_a}^{x_b} \rho A(x) dx = \frac{p}{R} \int_{x_a}^{x_b} \frac{A(x) dx}{T_w(x,t)}.
\]

In accordance with the temperature law (19)-(20), the analytic expression for the balance of mass flow through the ends with respect to the input mass flow \(m_{\text{bal,an}}\) is

\[
m_{\text{bal,an}} = -\frac{dM}{dt}/m_b = -\frac{2\pi a^2}{Q_{\text{inp}}} \int_0^t \frac{d}{dt} \left( \frac{T_0}{T_w(x,t)} \right) dx.
\]

The time-dependent profile of \(m_{	ext{bal,an}}\) for the input volume flow \(Q_{\text{inp}}=900\text{ml/min}\) is given on Fig. 4. In addition to evident sharp changes of \(m_{\text{bal,an}}\) at \(t=2\text{s}, 3\text{s}, 4\text{s}, 5\text{s}, 6\text{s}, 17\text{s}\) in accordance with the changes of the temperature law \(T_w(0,t)\), two time moments \(t=4.065\text{s}\) and \(15.653\text{s}\) exist where \(T_w(0,t)\) is equal to 600K; at these moments, in accordance with (19), for \(x\in[14, 16.8]\), the temperature law \(T_w(x,t)\) also sharply changes in time. This is the reason of the sharp change of \(m_{\text{bal,an}}\).

**TEMPERATURE DISTRIBUTIONS**

**PRESSURE AND VELOCITY DISTRIBUTIONS**

Figure 5: The pressure, velocity and temperature spatial distributions at time \(t=5.5\text{s}\)

On Fig. 4, one can see also the calculated value of \(m_{\text{bal,cal}}\)

\[
m_{\text{bal,cal}} = (m_a - m_b)/m_b,
\]

which is derived for \(x_a = -49\text{mm}, x_b = 36.8\text{mm}\) in accordance with the computation region shown on Fig. 7. One can see a satisfactory correlation between the analytic and computed
data which is better than in\textsuperscript{1}, because in the last paper the internal energy gradient at the tube wall was calculated with an error. For the time region between 2s and 3s, where the wall temperature slightly increases and, in the tube section, the temperature of gas has a time to accept the temperature of the wall, we see that the coincidence is better than that in the case of a rapid and large increase of the wall temperature with the time in the interval from 4s to 5s.

The above difference can also be explained by a significant convection flow which transfers over the temperature along the stream direction as one can see on Fig. 5, where the pressure, velocity, and temperature spatial distributions are presented for the time $t=5.5s$. For the sake of convenience, we restored the full domain of longitudinal section of the tube from the calculated axial symmetry part.

In the program, the values $\rho$, $I$, and $p$ are treated as those of double precision, meanwhile almost all remaining quantities (including the velocity $u$, geometric coefficients $c$ and $c'$, and the coordinates) are taken with the single precision. We take the following relations

$$\varepsilon_{\rho,l}=2\cdot10^{-5}, \varepsilon_u=0.3\cdot10^{-5}, \varepsilon_{u(P:\text{link})}=0.2\cdot10^{-3}$$

in the capacity of convergence criteria.

10 THEORETICAL TESTING OF THE METHOD. CONVERGENCE OF ITERATION SCHEME

The consistency of finite-difference equations for different kinds of geometrical coefficients follows from the analysis carried out in Sections 5.2 and 5.3.

With the use of the Newton method, a new numerical method previously published in\textsuperscript{1} for solving the three-dimensional Navier-Stokes equations is theoretically proved in this section for the most simple case of one-dimensional acoustic equations\textsuperscript{8}

$$\frac{\partial u}{\partial t} = a \frac{\partial v}{\partial x},$$

$$\frac{\partial v}{\partial t} = a \frac{\partial u}{\partial x}.$$ 

Here $v$ is a velocity with the opposite sign, $u$ is proportional to the pressure, $a$ stands for the sound speed. Further we will call $v$ the velocity and $u$ the pressure. The discretized equations with a weighted scheme with the weight $\omega$ are as follows

$$Q_v \equiv v^{j+1}_i - v^j_i - \gamma[(1-\omega)(u^j_i - u^j_{i-1}) + \omega(u^{j+1}_i - u^{j+1}_{i-1})], \quad Q_v = 0. \tag{21}$$

$$Q_u \equiv u^{j+1}_i - u^j_i - \gamma[(1-\omega)(v^j_i - v^j_{i+1}) + \omega(v^{j+1}_{i+1} - v^{j+1}_i)], \quad Q_u = 0. \tag{22}$$

Here $v_i$ stands for velocity value at the point $i$, $u_i$ is the pressure at the point $i+1/2$, $j$ corresponds to the time $t$, $j+1$ corresponds to the time $t+\Delta t$, $x_{i+1} - x_i = h$, $\gamma = a\Delta t/h$.

In\textsuperscript{8} the stability of the scheme (21), (22) was proved for $\omega \geq 0.5$. In correspondence with our method, let us construct the Newton-type iteration scheme and prove its stability along
with the convergence. We assume that we already know the values \( v_i^j, u_i^j \) for all \( i \). The values \( v_i^{j+1}, u_i^{j+1} \) are such that equations (21), (22) are fulfilled exactly. We will find these values by the iteration method. As in [8], we denote by \( v_i^k, u_i^k \) the values of \( v_i^{j+1}, u_i^{j+1} \) on the \( k \)-th iteration, respectively. In the capacity of initial guesses at the time \( t+\Delta t \), we take the values at the time \( t \)

\[
v_i^0 = v_i^j, \quad u_i^0 = u_i^j.
\]

We will determine further approximations by means of the Newton iteration procedure:

\[
v_i^{k+1} = v_i^k - \frac{Q_i^k}{\partial Q_i / \partial v_i^{j+1}}, \tag{23}
\]

\[
u_i^{k+1} = u_i^k - \frac{Q_u^k}{\partial Q_u / \partial u_i^{j+1}}. \tag{24}
\]

Here \( Q_i^k \) and \( Q_u^k \) are obtained from the expressions for \( Q_i \) and \( Q_u \) in formulas (21), (22) by means of the change of \( v_i^{j+1}, u_i^{j+1} \) by \( v_i^k, u_i^k \) for all \( i \). If by means of (23) we first determine \( v_i^{k+1} \) for all \( i \), then instead of (24) one can use

\[
u_i^{k+1} = u_i^k - \frac{Q_u^{k+1}}{\partial Q_u / \partial u_i^{j+1}}, \tag{25}
\]

where \( Q_u^{k+1} \) are obtained from the expression for \( Q_u \) in formula (22) due to the change of \( v_i^{j+1}, u_i^{j+1} \) by \( v_i^{k+1}, u_i^k \) for all \( i \).

In these formulas the values \( \partial Q_i / \partial v_i^{j+1} \) and \( \partial Q_u / \partial u_i^{j+1} \) denoted from a formal standpoint as partial derivatives of \( Q_i \) and \( Q_u \), respectively, are indeed treated by us as some factors really requiring in their determination the calculation of partial derivatives by the variables \( v_i^{j+1}, u_i^{j+1} \), which participate in explicit form in the expression for \( Q_i \) and \( Q_u \). However, these factors also may contain components due to other terms whose change is related by us (due to some reasons) to the change of the variables \( v_i^{j+1}, u_i^{j+1} \). We call these partial derivatives (as it was noted above) the correct rates of the change of residuals (CRCR). Clearly, the use of the term "Newton iteration method" is slightly conditional here. This means that we use this method here; however, a certain choice of artificial interrelations of variables may generate different iteration schemes. The traditional Newton method for various variables the equations for variables to be calculated for each iteration turn to be interrelated between each other and thus cannot be solved separately. In our case, oppositely, from one equation (or two equations: the energy equation and the continuity equation, as in the determination of the internal energy \( I \)), for the unknown at every point of the mesh we can obtain at once the desired unknown value at every point.
Let us find \( \partial Q / \partial u_i^{j+1} \). To this end, we relate \( \delta Q_u \) (i.e. the change of the residual \( Q_u \)) to \( \delta u_i^{j+1} \), i.e. the change of the \( u_i^{j+1} \). In doing so we assume that Eq. (21) is fulfilled and for \( v_i^{j+1} \) and for \( v_i^{j+1} + \delta v_i^{j+1} \) for all \( i \). In other words, we will assume that the increment \( \delta u_i^{j+1} \) implies a change \( \delta v_i^{j+1} \) such that Eq. (21) is fulfilled for \( v_i^{j+1} + \delta v_i^{j+1} \). Therefore, \( \delta Q_u = 0 \), whence it follows

\[
\delta v_i^{j+1} = \gamma \delta (\delta u_i^{j+1} - \delta u_{i-1}^{j+1})
\]

(26)

For the expression for \( Q_u \) in formula (22) we obtain

\[
\delta Q_u = \delta u_i^{j+1} - \gamma \omega (\delta v_i^{j+1} - \delta v_{i-1}^{j+1}).
\]

By substituting into it the expression (26) for \( i = i+1 \) and \( i = i \), we obtain

\[
\delta Q_u = \delta u_i^{j+1} - \gamma \omega (\delta u_i^{j+1} - 2\delta u_i^{j+1} + \delta u_{i-1}^{j+1}).
\]

Let

\[
\delta u_{i+1}^{j+1} = \omega(i,i+1)\delta u_i^{j+1}, \quad \delta u_{i-1}^{j+1} = \omega(i,i-1)\delta u_i^{j+1}.
\]

then we have

\[
\delta Q_u = \delta u_i^{j+1} \left[ 1 + 2\gamma \omega (1 - \omega(i,i+1) + \omega(i,i-1)) \right].
\]

Let us take \( \alpha(i,i+1) \) and \( \alpha(i,i-1) \) as constant values independent of \( i \) and equal to \( \omega_i(i,i) \); then we have

\[
\delta Q_u = \delta u_i^{j+1} \left[ 1 + 2\gamma \omega (1 - \omega_i(i,i)) \right].
\]

In the capacity of \( \partial Q_u / \partial u_i^{j+1} \) in formula (24) we take \( \partial Q_u / \partial u_i^{j+1} \); we then derive

\[
\partial Q_u / \partial u_i^{j+1} = 1 + 2\gamma \omega (1 - \omega_i(i,i)).
\]

(27)

In a similar way, we can obtain for \( \partial Q_u / \partial v_i^{j+1} \) in formula (23):

\[
\partial Q_v / \partial v_i^{j+1} = 1 + 2\gamma \omega (1 - \omega_i(i,i)).
\]

(28)

Let us investigate the iteration scheme (23), (24) with coefficients (27), (28) for the stability. To this end, as in \( ^8 \), we introduce the following notation

\[
\delta u_i^k = u_i^k - u_i^{j+1}, \quad \delta v_i^k = v_i^k - v_i^{j+1}.
\]

By subtracting in equation (24) from both the left-hand and right-hand sides the value \( u_i^{j+1} \) and by replacing \( Q_u \) by \( Q_u - Q_u \), where \( Q_u \) is defined by (22) and is equal to zero, we obtain
\[ \delta u_i^{k+1} = \delta u_i^k + \frac{\delta u_i^k - \gamma_0 (\delta v_{i+1}^{k+1} - \delta v_i^k)}{1 + 2\gamma^2 \omega^2 (1 - \omega_0)}. \]

whence it follows
\[ \delta u_i^{k+1} = \frac{2\gamma^2 \omega^2 (1 - \omega_0) \delta u_i^k + \gamma_0 (\delta u_i^k - \delta u_{i-1}^k)}{1 + 2\gamma^2 \omega^2 (1 - \omega_0)}. \]  

(29)

In a similar way, from (23) we obtain
\[ \delta v_i^{k+1} = \frac{2\gamma^2 \omega^2 (1 - \omega_0) \delta v_i^k + \gamma_0 (\delta v_i^k - \delta v_{i+1}^k)}{1 + 2\gamma^2 \omega^2 (1 - \omega_0)}. \]  

(30)

If instead of (23), (24) we use in our iteration scheme (23), (25), then instead of (29) we obtain
\[ \delta u_i^{k+1} = \frac{2\gamma^2 \omega^2 (1 - \omega_0) \delta u_i^k + \gamma_0 (\delta u_i^k - \delta u_{i-1}^k)}{1 + 2\gamma^2 \omega^2 (1 - \omega_0)}. \]  

(31)

As in \(^8\), we introduce the norms
\[ \| \delta u^k \| = \max_i |\delta u_i^k|. \]
\[ \| \delta v^k \| = \max_i |\delta v_i^k|. \]

If with \( \omega_0 = \omega = \omega_0 \leq 1 \) from (29), (30) one obtains estimates for the norms and then sums them, then the respective result is
\[ \| \delta u^{k+1} \| + \| \delta v^{k+1} \| \leq \frac{2\gamma^2 \omega^2 (1 - \omega_0) + 2\gamma_0 \omega}{2\gamma^2 \omega^2 (1 - \omega_0) + 1} (\| \delta u^k \| + \| \delta v^{k} \|). \]

Clearly, for large \( \gamma \), \( \gamma > \frac{1}{2\omega} \), this formula does not prove the stability of the scheme. The investigation under the same assumption ( \( \omega_0 = \omega = \omega_0 \leq 1 \) ) of formulas (30), (31) instead of (29), (30) is cumbersome and, seemingly, leads to the same result. The numerical experiment carried out already for the three-dimensional Navier-Stokes equations, shows that the convergence is observed only for small \( \gamma \sim 1 \).

Let us prove the convergence (stability) of another iteration scheme, where we use formulas (23) and (25), \( \partial Q_i/\partial u_i^{j+1} \) determine as earlier from formula (27), but now the coefficient \( \partial Q_i/\partial v_i^{j+1} \) is taken equal to 1. Instead of (30) we obtain a new relation if in (30) we replace \( \omega_0 \) by 1, because, in accordance with (28), \( \partial Q_i/\partial v_i^{j+1} \) appears as equal to 1 if in (28) we replace \( \omega_0 \) by 1

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\[ \delta v_i^{k+1} = \gamma \omega (\delta u_i^k - \delta u_{i-1}^k). \]  \hspace{1cm} (32)

By increasing the index \( i \) by 1, from (32) we obtain
\[ \delta v_i^{k+1} = \gamma \omega (\delta u_{i+1}^k - \delta u_i^k). \]  \hspace{1cm} (33)

and finally
\[ \delta v_{i+1}^{k+1} - \delta v_i^{k+1} = \gamma \omega (\delta u_{i+1}^k - 2\delta u_i^k + \delta u_{i-1}^k). \]

which after substitution into (31) gives us
\[ \delta u_i^{k+1} = \frac{\gamma^2 \omega^2 (\delta u_{i+1}^k + \delta u_{i-1}^k - 2\omega_0 \delta u_i^k)}{1 + 2\gamma^2 \omega^2 (1 - \omega_0)}. \]  \hspace{1cm} (34)

For \( \omega_{u0} \leq 1 \), from (34) we obtain
\[ \left| \delta u_i^{k+1} \right| \leq \frac{2\gamma^2 \omega^2 (1 + |\omega_{u0}|)}{2\gamma^2 \omega^2 (1 - \omega_{u0}) + 1} \| \delta u_i^k \| \]
whence
\[ \left\| \delta u_i^{k+1} \right\| \leq \frac{2\gamma^2 \omega^2 (1 + |\omega_{u0}|)}{2\gamma^2 \omega^2 (1 - \omega_{u0}) + 1} \| \delta u_i^k \|. \]  \hspace{1cm} (35)

Let us introduce the value \( \lambda \)
\[ \lambda = \frac{2\gamma^2 \omega^2 (1 + |\omega_{u0}|)}{2\gamma^2 \omega^2 (1 - \omega_{u0}) + 1}. \]

Then from (35) it follows
\[ \left\| \delta u_i^k \right\| \leq \lambda^k \left\| \delta u_i^0 \right\|. \]  \hspace{1cm} (36)

From (33) we have
\[ \left\| \delta v_{i+1}^{k+1} \right\| \leq 2\gamma \lambda \left\| \delta u_i^k \right\|. \]

and with regard for (36) we derive
\[ \left\| \delta v_i^{k+1} \right\| \leq 2\gamma \lambda^k \left\| \delta u_i^0 \right\|. \]  \hspace{1cm} (37)

From (36) and (37) it follows that, for \( \omega_{u0} \leq 0 \), when \( \lambda < 1 \), our iteration scheme converges for any \( \gamma \).

11 CONCLUSIONS

With the use of the Newton method, a new numerical iteration method previously
published in\textsuperscript{1} for solving the three-dimensional Navier-Stokes equations, is theoretically investigated in this paper for the most simple case of one-dimensional acoustic equations. The convergence of iteration scheme has been proved for any step in time, in particular, for the time step $\Delta t >> h/a$ (here $a$ is the sound speed).

In a numerical attempt, i.e. a posteriori in the process of calculation, the author succeeded in\textsuperscript{1} achieving the maximal time step $\Delta t_{\text{max}}=h/\text{u}_{\text{flow}}$ while keeping the number of arithmetic operations on the order of that of an explicit scheme.

The author expressed in\textsuperscript{1} a hope to develop in future the method in such a way that the time step $\Delta t$ would not be restricted by the value $h/\text{u}_{\text{flow}}$ and such $\Delta t$ would be reached during a lesser time of computation. However, the hope has not yet been materialised.

Seemingly, it is not reasonable to hope that the method will be developed solely by numerical computational experiments. Theoretic investigations of the convergence of iteration schemes and their modifications are necessary for more complex cases of approximation than that in the case of acoustic equations.

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