An explicit iterative scheme for 3D multicomponent heat conducting flow simulation

O.B. Feodoritova¹, N.D. Novikova¹ and V.T. Zhukov¹

¹Keldysh Institute of Applied Mathematics, RAS, 125047, Miusskaya sq. 4, Moscow, Russia
E-mail: feodor@kiam.ru, nn@kiam.ru, zhukov@kiam.ru

Abstract. This paper presents the development and testing of time integration scheme for the system of hydrodynamic equations of gas mixture. These equations take into account the phenomena of multicomponent diffusion and heat transfer. The governing equation system is discretized by the finite volume approach on three-dimensional unstructured grids. According to the algorithm, computation of any single time step is split into the sequence of hyperbolic and parabolic stages. The hyperbolic subtask is solved using the Godunov-type scheme. The parabolic subtask is solved by the explicit iterative Chebyshev scheme, which is algorithmically simple and does not involve tuning parameters. This stage addresses dissipative fluxes (viscosity, multicomponent diffusion and thermal conductivity). The number of the explicit iterations is determined by the convective time step and by the upper bound for the discrete diffusion operator. The resulting scheme ensures the fulfillment of the conservation laws at the discrete level. The computer code can be used in highly parallel computing for large-scale simulation. The proposed approach is recommended for applied problems in which convective and dissipative processes are in close interaction, particularly for problems of plasma physics and astrophysics.

1. Introduction

For numerical simulation of multicomponent flows we develop a new approach which demonstrates here in application to the three-dimensional equations of compressible heat conducting flows, see [1]. According to the proposed algorithm, computation of a single time step is split into the sequence of hyperbolic and parabolic stages. In the hyperbolic substep, we take into account the convective gasdynamic fluxes; in the parabolic substep the all dissipative fluxes are considered. The reason is that it is faster to solve the split terms separately, than to solve the multicomponent system directly. The additional advantage of the splitting approach is that the hyperbolic and the parabolic equations have different nature and they can be solved by different methods. In our splitting approach the hyperbolic subproblem is solved by the explicit Godunov’s type scheme [2]. Therefore, the time step size $\tau_{\text{conv}}$ is restricted by the convective stability condition. On parabolic stages we solve three diffusion subproblems which takes into account processes of viscosity, multicomponent diffusion and heat conduction. For diffusion-dominated process the usage of the explicit scheme is practically impossible. In this case, one might write an implicit scheme, which can be solved by an iterative algorithm. Usually such algorithms require empirical parameters. Instead of the implicit scheme we propose an explicit iterative LINS scheme [1] (Local Iterations for Navier-Stokes equations), which uses a special construction of Chebyshev polynomials. The LINS scheme inherits main properties of the LI-M scheme [3] and provides the fulfillment of the governing conservation laws.
In the LINS scheme there are not empirical parameters. The number of the explicit iterations is determined by the convective time step and the upper bound for the discrete diffusion operator.

The developed approach is recommended for problems in which convective and dissipative processes are in close interaction.

The objective of this paper is to present some new insights into an explicit iterative time integration approach, the LINS scheme, for hydrodynamic equations of multicomponent gas mixture. The paper is organized as follows. In Section 2 we present the governing equations. In Section 3 the general splitting algorithm is presented. In Section 4 we describe the time integration scheme for parabolic subtasks. In Section 5 a few test problems are described and their results are presented. Some conclusions are given in the last section.

2. The governing equations

We assume that a gas mixture consists of a set of chemical components with mass fractions $Y_m$, $m = 1, ..., N_{Sp}$, such as air or components of a hydrocarbon fuel. In this paper we take into account the phenomena of multicomponent diffusion and heat transfer. High-temperature phenomena (dissociation and ionization) will not be considered here. The description of turbulence and model of chemical interaction between components is omitted. Numerical simulations of such multicomponent flows are based on the system of Unsteady Reynolds averaged Navier-Stokes equations with the introduction of additional terms and equations for accounting for the effects of multicomponent diffusion, see, e.g., [4, 5]. It is assumed to sum up the repeated indexes $i, j = 1, 2, 3$ below.

Continuity equation:
\[
\frac{\partial \rho}{\partial t} + \sum \frac{\partial (\rho u_i)}{\partial x_i} = 0 .
\]  

Momentum conservation:
\[
\frac{\partial (\rho u_i)}{\partial t} + \sum \frac{\partial (\rho u_i u_j)}{\partial x_j} = - \frac{\partial p^*}{\partial x_i} + \sum \frac{\partial}{\partial x_j} [\tau_{ij}] .
\]  

Energy conservation:
\[
\frac{\partial (\rho E)}{\partial t} + \sum \frac{\partial (\rho u_j E + u_j p^*)}{\partial x_j} = - \sum \frac{\partial q^T_i}{\partial x_j} + \sum \frac{\partial}{\partial x_j} [u_i \tau_{ij}] .
\]  

The transfer equations of the components have the form:
\[
\frac{\partial (\rho Y_m)}{\partial t} + \sum \frac{\partial (\rho u_j Y_m)}{\partial x_j} = - \sum \frac{\partial J_{j,m}}{\partial x_j} + \dot{\omega}_m ,
\]  

and the following conditions are met
\[
\sum Y_m = 1, \quad \sum J_{j,m} = \sum \dot{\omega}_m = 0 .
\]  

Summation in these and similar formulas is based on the number of components from $m = 1$ to $N_{Sp}$. The equations (1)–(4) use the notations: $\vec{u} = \{u_i\}$ is the velocity vector of the averaged flow of a gas mixture; $\rho$ is the mixture density; $p^*$ is the thermodynamic pressure of the mixture, $E = e + 0.5 \cdot u_i u_i \equiv e + k$ is the total energy of multicomponent flow, $e$ is the specific internal energy, $k$ is the kinetic energy; $\vec{q}^T = \{q_i^T\}$ is the vector of flow caused by temperature changes; $J_{j,m}$, $q_i^T$ are the components of the diffusion and the heat fluxes respectively; $\tau_{ij}$ is the tensor of viscous stresses; $\dot{\omega}_m$ is the source term. The perfect gas model is used. The total heat flux consists of two parts: the actual heat flux and the diffusion flux of the mixture:
Here \( \lambda \) is the thermal conductivity of the mixture. The diffusion flux of each component is defined as \( J_{m,j} = -\rho D_m \cdot \partial Y_m / \partial x_j \), where \( D_m \) is the effective diffusion coefficient. Current state of the development is based on the simple convenient approach: for the molecular viscosity of each component the Sutherland formula is used, the thermal conductivity and diffusion coefficients of each component are taken as \( \lambda_m = C_{p,m}(T) \mu_m / \Pr \) and \( D_m = \mu_m / (\rho Sc) \), here \( C_{p,m}(T) \) is the component heat capacity at constant pressure, Prandtl number \( \Pr \) and Schmidt number \( Sc \) are given. To average the viscosity and thermal conductivity we use the formulas
\[
\mu = \frac{1}{2} \left[ \sum \mu_k X_k + \left( \sum \frac{X_k}{\mu_k} \right)^{-1} \right], \quad \lambda = \frac{1}{2} \left[ \sum \lambda_k X_k + \left( \sum \frac{X_k}{\lambda_k} \right)^{-1} \right],
\]
here \( X_k = Y_k M / M_k \), \( M_k \) and \( M \) are the molar masses of a component and mixture, respectively. The term \( \dot{\omega}_m \) responsible for chemical reactions is described in the standard way, see [4].

3. The numerical scheme
The system (1)–(4) are discretized in the integral form with conservative variables. The finite-volume node-based algorithm is employed for spatial discretization. Firstly the dual grid is constructed by forming non-overlapping elements, referred as dual cells, around each grid node. Integrating over each dual cell the semi-discrete scheme is written. We assume that the convective and diffusion fluxes are determined at dual cell interfaces. All the discrete constructions are based on the templates of the author’s package NOISEtte [6, 7]. As a result, the our new computer code MCFL (MultiComponent FLows) inherits the high parallel efficiency of the NOISEtte code.

We introduce the state vector \( U \equiv \rho (1, u_1, u_2, u_3, E, \{Y_m, m = 1, ..., N_{sp}\}) \) of conservative variables and write down the semidiscrete approximation of the system (1) – (4) as follows
\[
\frac{\partial}{\partial t} U + C_h(U) + D_h(U) = 0 ,
\]
where \( C_h \) is the nonlinear convective discrete operator on a spatial grid with a characteristic cell diameter \( h \), and \( D_h \) is the a nonlinear diffusive operator, associated with dissipative processes of viscosity, multicomponent diffusion and heat conduction. We assume that suitable boundary conditions are imposed at the boundary of a 3D domain which the formulated system is being solved, and these boundary conditions are included in the definitions of the scheme. Applying linearization to the equation (5), we write down an explicit scheme with a time step \( \tau \):
\[
\frac{U_{j+1} - U_j}{\tau} + C_h U_j + D_h U_j = 0 .
\]
Here, in (6), we do not introduce new notations for the linear operators \( C_h, D_h \) and omit a source of various origins. The linear operator \( D_h \) arises from approximation of a differential elliptic operator, therefore it is a non-negative definite self adjoint operator in the grid function space with appropriate boundary conditions. For the scheme (6) the time step \( \tau \) is restricted by the combined convective-diffusion stability condition. To overcome this restriction we propose an approach that preserves the time step constraint which corresponds only to the hyperbolic CFL condition. To do this we use the method of splitting the system into hyperbolic and diffusion parts. We solve the diffusion subproblem using a special explicit iterative process. In detail,
at each time step we implement two stages. At the first stage we set $D_h = 0$ and solve the intermediate discrete hyperbolic subproblem (corresponding to convective flows)

$$\frac{\bar{U}_j - U_j}{\tau} + C_h U_j = 0.$$  
(7)

On this stage the multicomponent modification of the Godunov scheme with the exact solution of the Riemann problem is used [2]. Thus, the state vector $\bar{U}_j$ is obtained at the hyperbolic stage as intermediate ones. At the second stage we set $C_h = 0$ and solve the discrete parabolic subproblem (corresponding to diffusion flows) with initial data $\bar{U}_j$

$$\frac{U_{j+1} - \bar{U}_j}{\tau} + D_h \hat{U}_j = 0.$$  
(8)

The parabolic subtask combines three parabolic subsystems which are taking into account viscosity, multicomponent diffusion and heat conduction. Each subsystem can be considered separately but we describe our computational scheme for the whole system.

In the scheme (8) one can take $U_j$ instead of $\hat{U}_j$, then the sum of (8) and (7) leads to the explicit scheme (6). As we know this scheme requires the diffusion restriction on the time step size, $\tau \sim h^2$. For diffusion-dominated process the usage of the explicit scheme with such time step restriction is practically impossible. In this case, one can write an implicit scheme, which can be solved by an iterative algorithm. Usually such algorithms require empirical settings (accuracy tolerance, preconditioned parameters, etc). Instead of an implicit scheme we propose a new explicit iterative scheme called LINS (Local Iterations for Navier-Stokes equations) introduced in [2]. It inherits basic properties of the LI-M scheme [3] and provides the fulfilment of the conservation laws for the entire system. The level-to-level transfer operator $Q_p (D_h)$ of this scheme represents a rational function of $D_h$. The transfer operator propagates an error from $t_j$ to $t_{j+1}$ and is defined by a Chebyshev polynomial. To construct desired polynomial we need to known only upper estimate of the operator $D_h$. This estimate is an evaluation of the maximal eigenvalue of the operator $D_h$ and this is obtained by the known Gershgorin theorem [8]. The time approximation and stability of the scheme are provided by a special choice of the Chebyshev polynomial. Due to the LINS algorithm the scheme (8) is equivalent to the final iteration of the LINS scheme. The number $q$ of the LINS iterations is determined by the degree

$$p = \left[0.25\pi \sqrt{\tau \lambda_{max} + 1}\right]$$  
(9)

of the Chebyshev polynomial as $q = 2p - 1$. Here the function $[s]$ is the smallest integer greater than or equal to $s$, $\lambda_{max}$ is an upper bound of the spectrum of the discrete operator $D_h$. The resulting algorithm remains stable under the hyperbolic time step restriction $\tau \sim const \cdot h$ and provides efficient parallelization.

For hyperbolic (convective) processes, the time step constraint is determined by the Courant–Friedrichs–Lewy (CFL) condition $a \tau / h \leq 1$, where $a$ is the velocity of propagation of perturbations in a cell of diameter $h$. A procedure for choosing $\tau_{conv}$ in the Godunov’s scheme can be found in [9]. We denote the maximum admissible step size as $\tau_{conv}$. Then the time step $\tau$ for computations is usually chosen so that $\tau \leq \tau_{conv}$. The ratio $Cu = \tau / \tau_{conv}$ is the hyperbolic Courant number.

The maximum time step for explicit diffusion computations can be estimated as $\tau_{dif} = \lambda_{max}^{-1}$, so that the step size is chosen according to the constraint $\tau_{dif} \cdot \lambda_{max} \leq 1$, which is twice as strong as that following from the well-known stability condition $-1 \leq 1 - \tau_{dif} \cdot \lambda_{max} \leq 1$, which is based on the estimated norm of the level-to-level transition operator. The condition $\tau \leq \min(\tau_{conv}, \tau_{dif})$ may be inefficient (see, e.g., [10]). Accordingly, to ensure the correct
transition from the LINS to the purely explicit scheme, we use the following sufficient condition for the stability of the upwind explicit scheme for the linear convection diffusion equation [11]:

\[ \tau \leq \left( \frac{1}{\tau_{\text{conv}}} + \frac{1}{\tau_{\text{dif}}} \right)^{-1}. \]

Introducing the diffusion Courant number \( Cd = \frac{\tau}{\tau_{\text{dif}}} \) we rewrite the above condition as

\[ \tau \cdot \left( \frac{1}{\tau_{\text{conv}}} + \frac{1}{\tau_{\text{dif}}} \right) \leq C_u + C_d \leq 1. \]

This condition holds, for example, if \( C_u \leq 0.5 \) and \( C_d \leq 0.5 \) are both satisfied. These relations hold if the step size for the explicit integration of the entire system is determined by the condition \( \tau \leq 0.5 \min(\tau_{\text{conv}}, \tau_{\text{dif}}) \).

4. Algorithm for the LINS scheme

1. General scheme.
   1.1 Find the time steps \( \tau_{\text{conv}} \) and \( \tau_{\text{dif}} \).
   1.2 If diffusion does not dominate, i.e. \( \tau_{\text{conv}} \cdot \lambda_{\text{max}} = \tau_{\text{conv}}/\tau_{\text{dif}} \leq 0.5 \), we set \( p = \lfloor 0.25 \pi \sqrt{\tau \lambda_{\text{max}}} + 1 \rfloor = 1 \), and the LINS computations automatically pass into the explicit scheme with the step \( \tau_{\text{conv}} \) for the entire system.
   1.3 If diffusion dominates, i.e., \( \tau_{\text{conv}}/\tau_{\text{dif}} > 0.5 \) then the hyperbolic and diffusion stages are computed with the step \( \tau_{\text{conv}} \), but, at the diffusion stage, \( q = 2p - 1 > 1 \) and the explicit iterations [3] (see item 2 below) are used to solve the parabolic system.

2. The explicit iterative algorithm for the equation \( u_t + D_h u = 0 \) (transfer from \( t_j \) to \( t_{j+1} \)).
   2.1. Find the upper bound \( \lambda_{\text{max}} \) of the spectrum of the operator \( D_h \) and determine the first-kind Chebyshev polynomial \( T_p(x) = \cos \left( p \arccos x \right) \), where the degree \( p \) defines in (9), \(-1 \leq x \leq 1\).
   2.2 The set \( \beta_m, m = 1, \ldots, p \) of roots of the Chebyshev polynomial

\[ K_p = \left\{ \cos \frac{2i - 1}{2p} \pi, i = 1, 2, \ldots, p \right\} \]

is ordered for stability (see [12]) so that is the first root \( z_1 = \beta_1 = \cos \left( 0.5 \pi / p \right) \). For the given ordered set \( \beta_m \in K_p \), find the parameters

\[ a_m = \frac{\lambda_{\text{max}}}{1 + z_1} (z_1 - \beta_m), \quad m = 1, \ldots, p. \]

The final set of iteration parameters consists of \( q = 2p - 1 > 1 \) numbers:

\[ \{ b_1, \ldots, b_q \} \equiv \{ a_p, \ldots, a_2, a_p, \ldots, a_2, a_1 \}. \]

In this set, the parameters \( a_p, \ldots, a_2 \) occur twice, while the parameter \( a_1 = 0 \), only once; the direct order can be used instead of the reverse one, which is of no matter.

2.3 Specify at the level \( j \) an initial approximation \( y^{(0)} = \bar{y}_j \), taken it from intermediate solution \( \bar{U}_j \) according to (7), set \( \tau = \tau_{\text{conv}} \) and compute:

\[ y^{(l)} = \frac{1}{1 + \tau b_l} \left( y^{(0)} + \tau b_l y^{(l-1)} - \tau D_h y^{(l-1)} \right), \quad l = 1, 2, \ldots, q, \]

\[ u_{j+1} = y^{(q)}. \]

The result is the function \( u_{j+1} \) at the upper level.

The choice of the Chebyshev parameters ensures that \( a_1 = 0 \), therefore at every time step the last iteration of (10) is equivalent to the use of the explicit scheme, which corresponds to a predictor–corrector scheme based on conservation laws.
5. Numerical tests
We demonstrated the capabilities of the LINS scheme for a few model problems.

Test 1. We consider the thermal convection problem described by the Navier–Stokes equations, namely, the determination of an unsteady one-component gas flow with constant heating on the boundary [13]. The statement of this problem and numerical results are given in [2]. Here we only present a brief description. We assume that the gas with constant initial density $\rho_0$, temperature $T_0$, and velocity $u_0$, $v_0$, is confined to a closed domain between two walls, one of which is heated to the temperature $T_1 > T_0$ which remains unchanged, while the other is supported at the constant temperature $T_0$. The task was to find the propagation of heat and the gas flow at the subsequent times. We considered a perfect gas with thermal conductivity and viscosity depending on temperature according to Sutherland’s law.

The computations were performed on a bounded time interval from the initial state until the waves of temperature, velocity, density, and pressure collided with the opposite wall. The initial-boundary value problem was considered in the two-dimensional domain $0 < x < 1$, $0 < y < 1$. For one-dimensional flow simulation, periodic conditions were set on the lower and upper boundaries of the domain. The boundary conditions on the vertical walls were specified as $u(0,t) = 0$, $u(1,t) = 0$, $T(0,t) = 10$, $T(1,t) = 1$. The initial conditions at $t = 0$ were $\rho(x,0) = 1$, $u(x,0) = 1$, $T(x,0) = 1$. For the chosen nondimensionalization, the equation of state took the form $p = \rho T$. The computations were performed on a sequence of rectangular grids with $N_x \times N_y$ cells. The number $N_x$ of steps in the direction $Ox$ was varied, while the number $N_y$ of steps in the direction $Oy$ remained unchanged (because it is one-dimensional problem). Fig.1 shows the dynamics of pressure waves until the collision with the opposite wall. Dimensionless pressure plots are given in six moments in time $t_i = 0.05 \cdot i$, $i = 1,...,6$, and are denoted by digits 1, 2, ..., 6.

![Figure 1. Test 1. Profiles of pressure at time $t_i = 0.05 \cdot i$, $i = 1,...,6$, denoted by 1, 2, ..., 6.](image_url)

At the time $t_6 = 0.3$ the perturbations reached the right cold wall. These results were produced by the LINS scheme on the grid $320 \times 10$ with the convective Courant number
\( Cu = 0.125 \) chosen for reasons of accuracy. With growing time, the number of LINS iterations increased from 9 to 15. We remark that condition, that a wave advances over one time step by at most one spatial step, holds at \( Cu = 0.5 \), but not more.

The computations on grids with the number of nodes in the direction equal to \( N_x = 160 \) and \( N_x = 320 \) yield nearly identical results. On the grid with \( N_x = 320 \), the computational time required for LINS with \( \tau = 5 \cdot 10^{-4} \) is five times less than for an explicit scheme. With an increase in the number \( N_x \), the superiority of LINS scheme increases.

Test 2. We compute the 2D supersonic flow in a channel of variable cross section [14], see Fig. 2. We consider the steady flow of a viscous heat conducting one-component gas described by the Navier–Stokes equations. The channel length is chosen so that there is no recirculation flow in the outlet cross section at a given Reynolds number. Test computations on different grids were performed for a channel with adiabatic walls at the inlet Mach number \( M_\infty = 4 \) and the Reynolds number \( Re = 10^4 \) (which was computed using freestream parameters and the characteristic length which is specified by the distance from the axis of symmetry to the channel wall at the inlet).

![Figure 2. Test 2. Geometry of the channel](image)

The computations were performed on three grids with the total number of nodes given by \( N = 10^4, 4 \cdot 10^4, 16 \cdot 10^4 \). The indicated grids are adopted to all boundary layers: the dimensionless parameter characterizing the distance from the wall to the first grid node was varied along the wall in the range \( 0.1 \div 1 \), i.e., the boundary layer was well resolved.

The numerical results confirmed the flow features obtained in [14] for the steady laminar flow under study. The flow has a rather complex structure including interacting shock waves and expansion fans. To illustrate the structure of laminar steady flow Fig. 3 we show the density, relative units \( \rho/\rho_\infty \). A thick boundary layer with a flow separation zone is formed on the walls of the channel. The emergence of the separation zone is caused by the shock wave reflected from the axis (plane) of symmetry.

The LINS scheme works well. On the grid with \( N = 16 \cdot 10^4 \) the number of LINS iterations is equal to 7 – 9, depending on the convective step size. Under mesh refinement, the number of iterations increases (roughly in inverse proportion to the square root of the mesh size), but not drastically.
Test 3. We simulate 1-D acoustic propagation generated by the diffusion of inert $H_2 - O_2$ interfaces. This test case is implemented to show the performance of the proposed LINS scheme for the pressure wave production due to a density interface. The test is based on the work [15], with a slight modification. At $t_0 = 0$ a hydrogen spot with a top hat shape is located in the center of an oxygen medium. Temperature and pressure are uniform and the flow is at rest. When the species begin to diffuse, at each interface a pair of pressure waves set up in opposite directions. The first waves travel outward at sound velocity in the oxygen medium. Waves traveling faster into the hydrogen are partly transmitted through the opposite interface and partly reflected by this interface.

**Initial data.** At time $t = 0$ we set initial values of pressure, temperature, velocity: $p = \rho_0 = 1$ atm, $u = u_0 = 0$, $T = T_0 = 850$ K. We designate $L_1 = 0.5 \cdot (L_x - \Delta_0)$, $L_2 = 0.5 \cdot (L_x + \Delta_0)$, where $L_x = 0.04$ m, $\Delta_0 = 0.02$ m. For the component $Y_1$, oxygen medium, the distribution is set in the form of a discontinuous function, “a top hat shape”: $Y_1 = 1$, $L_1 < x < L_2$, and $Y_1 = 0$, $0 < x < L_1$, or $L_2 < x < 1$, the hydrogen concentration is $Y_2 = 1 - Y_1$.

**Boundary conditions.** The time interval at which pressure waves from density interfaces located at $x = 0.01$ and $x = 0.03$, do not reach external boundaries is considered. Therefore, at all four boundaries, one can set periodic boundary conditions, or along the $Ox$ axis, take the boundary conditions as $u(0, t) = 0$, $u(L_x, t) = 0$, $T(0, t) = T_0$, $T(L_x, t) = T_0$.

**Grids.** Calculations are carried out up to time $t_1 = 3.3464e - 06$ s on a sequence of uniform grids with the number of nodes $N = 400, 4000, 16000$ along the axis $Ox$ and a small number of nodes along the axis $Oy$ on which the solution is constant. For a grid with nodes $N = 4000$ we set time step $\tau \approx 3.85e - 10$ . This grid is chosen as sufficient for visualizing the calculations and discussing them, but for a more accurate simulation of acoustic waves and mixing zones, such calculations were made on more detailed grids, up to 32,000 nodes. With the coarse grids, the numerical diffusion of the acoustic waves is too high. The speed of sound is 550 m/s and 2200 m/s for oxygen and hydrogen, respectively, under conditions $p = 1$ atm, $T = 850$ K. If the dissipative terms are zero, then the state of rest is not disturbed. Due to the symmetry we describe the evolution of the initial discontinuity at the first initial oxygen-hydrogen boundary $x = 0.01$. In the presence of diffusion, a contact interface occurs here becomes smooth over time. The left and right acoustic waves run with speeds 550 m/s and 2200 m/s respectively in opposite
directions. In Fig. 4 and 5 the profiles of the velocity $m/s$ and mass fraction of hydrogen are shown in the mixing $O_2 − H_2$ zone at the final time; two acoustic waves running left and right are visible.

![Figure 4](image1.png)

**Figure 4.** Test 3. Velocity $m/s$ and mass fraction of hydrogen: left wave and mixing zone.

![Figure 5](image2.png)

**Figure 5.** Test 3. Velocity $m/s$ and mass fraction of hydrogen: mixing zone and right wave.
6. Conclusion
This article presents the time integration scheme for multicomponent gas mixture equations. The scheme has a few attractive features: the convection subproblem is solved explicitly by the robust Godunov-type algorithm, the diffusion subproblem is self-adjoint and solved by the efficient explicit iterative algorithm. On the diffusion substep the scheme does not require any tuning parameter. The code can be used in highly parallel computing for large-scale multicomponent simulation. Numerical experiments verify efficiency of this approach. The tested code appears to be a reliable tool for simulation of multicomponent flows. For this study, we used empirical approximations of the kinetic coefficients to show the capacities of this scheme. Applying this approach with more sophisticated models is straightforward. Extension to three-dimensional reactive multicomponent flows with unstructured grids and to simulation thermal interaction of a multicomponent flow with a solid body are under development.

The proposed technique is recommended for solving applied problems in which convective and dissipative processes are in close interaction, particularly for problems of plasma physics and astrophysics.

References
[1] V.T. Zhukov, N.D. Novikova, O.B. Feodoritova. An approach to time integration of the Navier-Stokes equations. // Comp. Mathematics and Math. Physics. 2020. V. 60. No. 2. P. 272-285.
[2] V.E. Borisov and Yu.G. Rykov. Modified Godunov Method for Multicomponent Flow Simulation. // J. Phys.: Conf. Ser. 1250 012006, 2019, doi:10.1088/1742-6596/1250/1/012006
[3] V.T. Zhukov. On explicit methods for the time integration of parabolic equations. // Math. Models Comput. Simul. 2011. V. 3. No. 3. P. 311–332.
[4] V.E. Borisov, O.B. Feodoritova, N.D. Novikova, Yu.G. Rykov, V.T. Zhukov. Computational Model for High-Speed Multicomponent Flows. // Mathematica Montisnigri. 2020. V. XLVIII. doi:10.20948/mathmontis-2020-48-4
[5] T. Poinsot, D. Veynante. Theoretical and numerical combustion. Edwards, 3rd Edition. 2011.
[6] I.V. Abalakin, P.A. Bakhvalov, A.V. Gorobets, A.P. Duben, T.K. Kozubskaya. Parallel research code NOISEtte for large-scale CFD and CAA simulation. // Num. Meth. Prog. 2012. V. 13. No. 3. P. 110–125. [in Russian]
[7] http://caa.imamod.ru/index.php/research/noisette
[8] F.R. Gantmacher. The Theory of Matrices. Chelsea, New York. 1959.
[9] Numerical Solution of Multidimensional Problems in Gas Dynamics, Ed. by S.K. Godunov, A.V. Zabrodin, M.Ya. Ivanov, A.N. Kraiko and G P. Prokopov. Nauka, Moscow. 1976. [in Russian].
[10] V.V. Vlasenko, Doctoral Dissertation in Physics and Mathematics. Central Aerodynamic Inst., Zhukovskii. 2017. [in Russian]
[11] A.A. Samarskii and P.N. Vabishchevich. Numerical Methods for Solving Convection–Diffusion Problems. URSS. Moscow. 1999. [in Russian].
[12] V.I. Lebedev and S.A. Finogenov. The order of choice of iteration parameters in the cyclic Chebyshev iteration method. // USSR Comput. Math. Math. Phys. 1971. V. 11. No. 2. P. 155–170.
[13] V.I. Polezhaev. Candidate’s Dissertation in Engineering, Research Inst. of Precision Instruments. Moscow. 1967. [in Russian].
[14] V.A. Bashkin and I.V. Egorov, Numerical Study of Exterior and Interior Aerodynamic Problems. Fizmatlit, Moscow. 2013. [in Russian].
[15] G. Billet, R. Abgrall. An Adaptive Shock-Capturing Algorithm for Solving Unsteady Reactive Flows. // Computers and Fluids. 2003. V. 32. No. 10. P. 1473–1495.