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An effective numerical method for simulating chemically and thermally nonequilibrium gas flows

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Abstract. A new efficient implicit numerical method has been developed for solving the equations of compressible viscous chemically and thermally nonequilibrium gas flow on structured grids. In this method, the problem of stiff is completely solved (the scheme is unconditionally stable), the number of matrix inversions is reduced, and the matrices themselves are factorized into smaller ones, and their inversion requires significantly less computer resources than for a fully implicit scheme. High convergence rate is achieved due to the fact that the algorithm can significantly reduce the decomposition errors of the approximate matrix in two ways. Test calculations were carried out, which showed a high efficiency of the proposed numerical schemes.

1. Introduction

Nowadays, aviation and rocket & space technology is undergoing another round of evolutionary development, for it poses fundamentally new tasks for both high-speed and safe flight in the atmosphere, as well as challenges for the development of near-Earth space and deep space.

The concept of complex mathematical modeling has become crucial in solving a number of problems in aviation and rocket & space technology, including the multiparameter problem of calculating the characteristics of highly enthalpy turbulent flows with nonequilibrium physicochemical processes.

The complexity of this task lies in the need to take into account thermodynamic nonequilibrium processes: nonequilibrium chemical reactions, thermal and dynamic nonequilibrium between different phases of the flow, thermal nonequilibrium between different degrees of freedom of gas molecules, as well as nonequilibrium development of turbulent mixing processes.

In gas flows, in which nonequilibrium chemical reactions and nonequilibrium energy transitions occur, the characteristic times of the main processes can vary by 10^4 - 10^6 times. In this case, the system of governing equations is stiff, and its direct numerical solution requires huge computer resources.

As a rule, implicit schemes are used to solve the stiffness problem. However, when a system of equations describes complex kinetic processes, including numerous chemical reactions and transitions between different energy modes, this system can include tens or even hundreds of equations. The use of standard implicit methods requires multiple inversions of matrices having a dimension corresponding to the number of equations at every time step in each node of the grid.

In this paper, we propose an effective implicit numerical method, in which, on the one hand, the stiffness problem is completely solved (the scheme is unconditionally stable); on the other hand, the number of matrix inversions is reduced, and the matrices themselves are factorized into smaller ones, so their inversion requires significantly less computer resources than in a standard implicit scheme.



2. Implicit matrix equations

Let us consider the unsteady equations of viscous chemically and thermally nonequilibrium gas flow represented in general coordinates ξ, η, ζ as follows

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{E}}{\partial \xi} + \frac{\partial \mathbf{F}}{\partial \eta} + \frac{\partial \mathbf{G}}{\partial \zeta} = \mathbf{H} \quad (1)$$

The system is written in vector form; it is solved relative to the state vector \mathbf{U} and includes the equations of continuity, momentum, total energy, rotational energy, vibrational energies, electron energy, conservation of species mass, etc. Vectors $\mathbf{E}, \mathbf{F}, \mathbf{G}$ describe the viscous and inviscid fluxes in these equations, and vector \mathbf{H} describes the sources.

The finite-volume approximation of equation (1), written in *delta law* form [1], is given by the following equation:

$$\left\{ I - \Delta t \left(\frac{\partial \mathbf{H}}{\partial \mathbf{U}} \right)_{i,j,k}^n + \Delta t \left(\frac{D_{-}}{\Delta \xi} \bar{\mathbf{A}}_{i+1/2,j,k}^n + \frac{D_{-}}{\Delta \eta} \bar{\mathbf{B}}_{i,j+1/2,k}^n + \frac{D_{-}}{\Delta \zeta} \bar{\mathbf{C}}_{i,j,k+1/2}^n \right) \right\} \delta \mathbf{U}_{i,j,k}^{n+1} = \Delta \mathbf{U}_{i,j,k}^n, \quad (2)$$

where $\delta \mathbf{U}^{n+1} = \mathbf{U}^{n+1} - \mathbf{U}^n$ is the change of the solution during the interval from time $n\Delta t$ to time $(n+1)\Delta t$; $\Delta \mathbf{U}_{i,j,k}^n$ is an explicit increment of this vector:

$$\Delta \mathbf{U}_{i,j,k}^n = \Delta t \mathbf{H}_{i,j,k}^n - \frac{\Delta t}{\Delta \xi} (\mathbf{E}_{i+1/2,j,k}^n - \mathbf{E}_{i-1/2,j,k}^n) - \frac{\Delta t}{\Delta \eta} (\mathbf{F}_{i,j+1/2,k}^n - \mathbf{F}_{i,j-1/2,k}^n) - \frac{\Delta t}{\Delta \zeta} (\mathbf{G}_{i,j,k+1/2}^n - \mathbf{G}_{i,j,k-1/2}^n) \quad (3)$$

$\bar{\mathbf{A}}, \bar{\mathbf{B}}$ and $\bar{\mathbf{C}}$ are Jacobi matrices of the flux vectors \mathbf{E} , \mathbf{F} , and \mathbf{G} with respect to the state vector \mathbf{U} , respectively; the dots \bullet appearing in the equation indicate the fact that difference operators operate on all factors to the right. When applying difference operators using Roe method [2] for splitting inviscid fluxes and Tysinger and Caughey approach [3] for implicit viscous fluxes, we obtain a system of equations of the following form

$$\begin{aligned} & \mathbf{A}_{i,j,k} \delta \mathbf{U}_{i,j,k}^{n+1} + \mathbf{B}_{i,j,k} \delta \mathbf{U}_{i,j+1,k}^{n+1} + \mathbf{C}_{i,j,k} \delta \mathbf{U}_{i,j-1,k}^{n+1} + \mathbf{D}_{i,j,k} \delta \mathbf{U}_{i+1,j,k}^{n+1} + \mathbf{E}_{i,j,k} \delta \mathbf{U}_{i-1,j,k}^{n+1} \\ & + \mathbf{F}_{i,j,k} \delta \mathbf{U}_{i+1,j,k}^{n+1} + \mathbf{G}_{i,j,k} \delta \mathbf{U}_{i-1,j,k}^{n+1} = \Delta \mathbf{U}_{i,j,k}^n \end{aligned} \quad (4)$$

where $\mathbf{A}_{i,j,k}, \mathbf{B}_{i,j,k}, \mathbf{C}_{i,j,k}, \mathbf{D}_{i,j,k}, \mathbf{E}_{i,j,k}, \mathbf{F}_{i,j,k}, \mathbf{G}_{i,j,k}$ are block matrix elements.

To solve the system (4), the effective MAF(k) McCormack method [1] can be used. The matrix of the system is decomposed (factorized) into the product of three tridiagonal matrices, each of which is solved using Thomas algorithm for block matrices.

This algorithm requires multiple inversions of matrices whose order is equal to the dimension of vector \mathbf{U} . In the case of a large number of equations included in system (1), that can lead to enormous expenditures of computer resources.

The fact is that source vector \mathbf{H} is associated with transitions between different energy modes, species rates of formation, sources in the equations of the turbulence model, etc. The time scales of these processes are very small and can lead to the system of equations becoming extremely stiff. The cost of using a completely implicit approach includes expensive time steps and complex coding. Suppose, for example, that a turbulent flow of a thermochemically nonequilibrium gas contains 14 species (H, O, OH, H₂, O₂, H₂O, N₂, CO, CO₂, H₂O₂, HO₂, NO, HCl, e⁻), there are 12 vibrational modes (CO, CO₂(v2), CO₂(v3), N₂, H₂O(v1), H₂O(v2), H₂O(v3), H₂, O₂, NO, OH, HCl) and 1 rotational mode and electron energy. In this case, we have a system of 34 equations: 1 continuity equation, 3 momentum equations, 1 total energy equation, 13 species conservation equations, 12 vibrational energy equations, 1 rotational energy equation, 1 electron energy equation and 2 turbulence model equations. For this particular formulation, block tri-diagonal solutions are required, where each block order is 34x34. Direct inversion of such matrices requires significant computer resources. The price of a large set of equations and a completely implicit approach is high memory demand.

It is necessary to find ways to simplify the solution of the implicit system (4).

3. Numerical method

First of all, we note that in equation (4) the block matrix elements $\mathbf{B}_{i,j,k}$, $\mathbf{C}_{i,j,k}$, $\mathbf{D}_{i,j,k}$, $\mathbf{E}_{i,j,k}$, $\mathbf{F}_{i,j,k}$, $\mathbf{G}_{i,j,k}$ are expressed only in terms of Jacobi matrices $\bar{\mathbf{A}}$, $\bar{\mathbf{B}}$ and $\bar{\mathbf{C}}$, which, as already mentioned, are associated with viscous/inviscid fluxes. In its turn, matrix $\mathbf{A}_{i,j,k}$ can be represented as

$$\mathbf{A}_{i,j,k} = \mathbf{I} + \alpha \Delta t \mathbf{a}_{i,j,k} - \alpha \Delta t \left(\frac{\partial \mathbf{H}}{\partial \mathbf{U}} \right)_{i,j,k}^n, \quad (5)$$

where matrix $\mathbf{a}_{i,j,k}$ is also a function of only viscous/inviscid fluxes. Here is $\alpha \geq 0.5$ is a parameter characterizing the order of accuracy of the time derivative.

Let us partition vector \mathbf{U} into 2 qualitatively different parts. The first one is basic and relates to the equations of continuity, conservation of momentum and conservation of total energy. Let us assume that N_b is a number of equations related to the first part; $N_b=5$ is for a three-dimensional case; $N_b=4$ is for a two-dimensional one.

The second part of vector \mathbf{U} refers to the additional equations: conservation of species, vibrational energies, etc. Let us assume that N_a is the total number of these additional equations.

The energy equation can be written via the total energy or via thermodynamic energy that does not include the chemical component of energy [4]. In the latter case, there appears a source on the right side of the energy equation, due to chemical reactions.

The analysis of the equations shows that, when using thermodynamic energy, the vectors of viscous/inviscid fluxes included in the first N_b equations are mainly the functions of only first N_b components of vector \mathbf{U} , being very slightly dependent on the rest of its components.

In its turn, the vectors of viscous/inviscid fluxes included in the additional equations depend on the first N_b components of vector \mathbf{U} and on its own component of this vector.

Thus, Jacobi matrices $\bar{\mathbf{A}}$, $\bar{\mathbf{B}}$, $\bar{\mathbf{C}}$ and, accordingly, the block matrix elements $\mathbf{B}_{i,j,k}$, $\mathbf{C}_{i,j,k}$, $\mathbf{D}_{i,j,k}$, $\mathbf{E}_{i,j,k}$, $\mathbf{F}_{i,j,k}$, $\mathbf{G}_{i,j,k}$, $\mathbf{a}_{i,j,k}$ can be represented in the following form

$$\Phi = \begin{pmatrix} \Phi_{11} & \Phi_{12} \\ \Phi_{21} & \Phi_{22} \end{pmatrix} = \begin{pmatrix} \Phi_{11} & \mathbf{0} \\ \Phi_{21} & \mathbf{D} \end{pmatrix}, \quad (6)$$

where the matrix blocks have the following orders: Φ_{11} - $N_b \times N_b$; Φ_{21} - $N_a \times N_b$; \mathbf{D} - diagonal matrix of size N_a .

We can introduce average special heat ratio $\bar{\gamma} = h^T / e^T$. This parameter is rather inertial, and when solving systems it changes only slightly depending on both spatial coordinates and time. Here h^T, e^T is the thermodynamic parts of the enthalpy and internal energy, respectively.

In that case, blocks Φ_{11} of all Jacobi matrices $\bar{\mathbf{A}}$, $\bar{\mathbf{B}}$, $\bar{\mathbf{C}}$ have exactly the same form as full Jacobi matrices in the case of a thermally perfect gas which is described by a system of N_b equations.

The main advantages of a matrix of the form (6):

1) its inversion is reduced to a single inversion of matrix Φ_{11} and trivial operations of matrix multiplication (Frobenius formula):

$$\Phi^{-1} = \begin{pmatrix} \Phi_{11}^{-1} & \mathbf{0} \\ -\mathbf{D}^{-1} \Phi_{21} \Phi_{11}^{-1} & \mathbf{D}^{-1} \end{pmatrix} \quad (7)$$

2) any necessary operations with such a matrix (inversion, multiplication) do not change its shape, i.e. block Φ_{12} remains zero, and block Φ_{22} remains a diagonal matrix.

In the case when the source vector $\mathbf{H} = \mathbf{0}$, the block matrix element $\mathbf{A}_{i,j,k}$ also has the form (6). In this case, even a significant increase in the number of additional equations does not lead to significant computer resources.

Unfortunately, all the advantages of using a matrix of the form (6) disappear in the presence of a nonzero source \mathbf{H} .

Therefore, instead of a direct numerical solution of system (4), it is proposed to use its approximation factorization.

We partition matrix $\partial\mathbf{H}/\partial\mathbf{U}$ into diagonal and off-diagonal components:

$$\partial\mathbf{H}/\partial\mathbf{U} = \mathbf{T} + \mathbf{d} \quad (8)$$

Let us consider a two-dimensional problem to reduce the record. It is not difficult to extend the method to a three-dimensional problem.

We consider the following two approximation schemes:

1) Approximate factorization 1

$$\left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \right] \left[\left(\mathbf{I} + \alpha\Delta t \mathbf{a}_{i,j} - \alpha\Delta t \mathbf{d}_{i,j}^n \right) \delta\mathbf{U}_{i,j}^{n+1} + \mathbf{B}_{i,j} \delta\mathbf{U}_{i,j+1}^{n+1} + \mathbf{C}_{i,j} \delta\mathbf{U}_{i,j-1}^{n+1} + \mathbf{D}_{i,j} \delta\mathbf{U}_{i+1,j}^{n+1} + \mathbf{E}_{i,j} \delta\mathbf{U}_{i-1,j}^{n+1} \right] = \Delta\mathbf{U}_{i,j}^{n+1} \quad (9)$$

2) Approximate factorization 2

$$\left[\mathbf{I} - \alpha\Delta t \left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}} \right)_{i,j}^n \right] \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \times \quad (10)$$

$$\times \left[\left(\mathbf{I} + \alpha\Delta t \mathbf{a}_{i,j} - \alpha\Delta t \mathbf{d}_{i,j}^n \right) \delta\mathbf{U}_{i,j}^{n+1} + \mathbf{B}_{i,j} \delta\mathbf{U}_{i,j+1}^{n+1} + \mathbf{C}_{i,j} \delta\mathbf{U}_{i,j-1}^{n+1} + \mathbf{D}_{i,j} \delta\mathbf{U}_{i+1,j}^{n+1} + \mathbf{E}_{i,j} \delta\mathbf{U}_{i-1,j}^{n+1} \right] = \Delta\mathbf{U}_{i,j}^{n+1}$$

From equation (9) it follows:

$$\left(\mathbf{I} + \alpha\Delta t \mathbf{a}_{i,j} - \alpha\Delta t \left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}} \right)_{i,j}^n - (\alpha\Delta t)^2 \mathbf{T}_{i,j}^n \mathbf{a}_{i,j} + (\alpha\Delta t)^2 \mathbf{T}_{i,j}^n \mathbf{d}_{i,j}^n \right) \delta\hat{\mathbf{U}}_{i,j}^{n+1} + \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \right] \mathbf{B}_{i,j} \delta\mathbf{U}_{i,j+1}^{n+1} \quad (11)$$

$$+ \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \right] \mathbf{C}_{i,j} \delta\mathbf{U}_{i,j-1}^{n+1} + \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \right] \mathbf{D}_{i,j} \delta\mathbf{U}_{i+1,j}^{n+1} + \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \right] \mathbf{E}_{i,j} \delta\mathbf{U}_{i-1,j}^{n+1} = \Delta\mathbf{U}_{i,j}^{n+1}$$

The coefficient at $\delta\mathbf{U}_{i,j}^{n+1}$ differs from the corresponding coefficient in (4) by a second-order value relative to Δt , and this value can be neglected. As a rule, diagonal elements play a decisive role in the matrix $\partial\mathbf{H}/\partial\mathbf{U}$, and assuming that

$$\alpha\Delta t \left\| \tilde{\mathbf{T}} \right\| \ll 1 \quad (12)$$

the scheme (11) is reduced to an initial implicit scheme (4).

Let us analyze the scheme (10):

$$\left\{ \mathbf{I} - \alpha\Delta t \left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}} \right)_{i,j}^n + \alpha\Delta t \mathbf{a}_{i,j} - (\alpha\Delta t)^2 \mathbf{T}_{i,j}^n \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \mathbf{a}_{i,j} \right\} \delta\mathbf{U}_{i,j}^{n+1} + \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \right] \mathbf{B}_{i,j} \delta\mathbf{U}_{i,j+1}^{n+1} \quad (13)$$

$$+ \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \right] \mathbf{C}_{i,j} \delta\mathbf{U}_{i,j-1}^{n+1} + \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \right] \mathbf{D}_{i,j} \delta\mathbf{U}_{i+1,j}^{n+1}$$

$$+ \left[\mathbf{I} - \alpha\Delta t \mathbf{T}_{i,j}^n \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \right] \mathbf{E}_{i,j} \delta\mathbf{U}_{i-1,j}^{n+1} = \Delta\mathbf{U}_{i,j}^{n+1}$$

And again, the coefficient at $\delta\mathbf{U}_{i,j}^{n+1}$ differs from the corresponding coefficient in (4) by a second-order value relative to Δt . In addition, if diagonal elements play a decisive role in the matrix $\partial\mathbf{H}/\partial\mathbf{U}$, then

$$\left\| \alpha\Delta t \mathbf{T}_{i,j}^n \left(\mathbf{I} - \alpha\Delta t \mathbf{d}_{i,j}^n \right)^{-1} \right\| = \left\| \mathbf{T}_{i,j}^n \left(\mathbf{I} / (\alpha\Delta t) - \mathbf{d}_{i,j}^n \right)^{-1} \right\| = \frac{\left\| \mathbf{T}_{i,j}^n \right\|}{\left\| \mathbf{I} / (\alpha\Delta t) - \mathbf{d}_{i,j}^n \right\|} \ll 1 \quad (14)$$

Thus, with sufficient accuracy, the equation (13) is transformed into

$$\left\{ \mathbf{I} - \alpha\Delta t \left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}} \right)_{i,j}^n + \alpha\Delta t \mathbf{a}_{i,j} \right\} \delta\mathbf{U}_{i,j}^{n+1} + \mathbf{B}_{i,j} \delta\mathbf{U}_{i,j+1}^{n+1} + \mathbf{C}_{i,j} \delta\mathbf{U}_{i,j-1}^{n+1} + \mathbf{D}_{i,j} \delta\mathbf{U}_{i+1,j}^{n+1} + \mathbf{E}_{i,j} \delta\mathbf{U}_{i-1,j}^{n+1} = \Delta\mathbf{U}_{i,j}^{n+1} \quad (15)$$

This expression exactly matches the implicit scheme (4).

Thus, the numerical scheme (10) is the most successful factorization of the main implicit scheme (4).

The solution of systems (9) and (10) is not very difficult. For example, for (9) we get:

$$\begin{aligned} & (\mathbf{I} + \alpha \Delta t \mathbf{a}_{i,j} - \alpha \Delta t \mathbf{d}_{i,j}^n) \delta \mathbf{U}_{i,j}^{n+1} + \mathbf{B}_{i,j} \delta \mathbf{U}_{i,j+1}^{n+1} + \mathbf{C}_{i,j} \delta \mathbf{U}_{i,j-1}^{n+1} + \mathbf{D}_{i,j} \delta \mathbf{U}_{i+1,j}^{n+1} + \mathbf{E}_{i,j} \delta \mathbf{U}_{i-1,j}^{n+1} \\ & = [\mathbf{I} - \alpha \Delta t \mathbf{T}_{i,j}^n]^{-1} \Delta \mathbf{U}_{i,j}^{n+1} \equiv \mathbf{X} \end{aligned} \quad (16)$$

The solution to this system is not different from the solution to the system (4) in the case of a zero source, because the diagonal matrix \mathbf{d} also corresponds to form (6). The inversion of the matrix $[\mathbf{I} - \alpha \Delta t \mathbf{T}_{i,j}^n]^{-1}$ is performed once at each time step and is not related to the block tridiagonal matrix algorithm. In addition, $\mathbf{T}_{i,j}^n$ is easily divided into blocks in accordance with physical processes. The inversion of these blocks is carried out separately and independently of each other.

4. Calculation results

To test the numerical model, we calculated several model supersonic jets mixing with the atmosphere.

4.1. Test 1

The conditions at the nozzle exit (the temperature, velocity, pressure, mole fractions of gas components) and the nozzle radius chosen for the calculation are shown in the Table 1.

Table 1. Conditions at the nozzle exit plane

p_a , Pa	T_a , K	U_a , m/s	R_a , m	X_{H_2}	X_{H_2O}	X_{CO}	X_{CO_2}	X_{N_2}
1×10^5	1330	2500	1.0	0.4	0.05	0.15	0.05	0.35

The parameters of the air coflow are: $p_e = 0.25 \times 10^5$ Pa, $T_e = 217$ K, $U_e = 300$ m/s.

The calculations took into account the chemical reactions involving the following species: H, O, OH, H₂, O₂, H₂O, N₂, CO, CO₂, H₂O₂, HO₂, NO.

Figure 1 shows the results of calculating jet centerline temperature variations using various numerical methods.

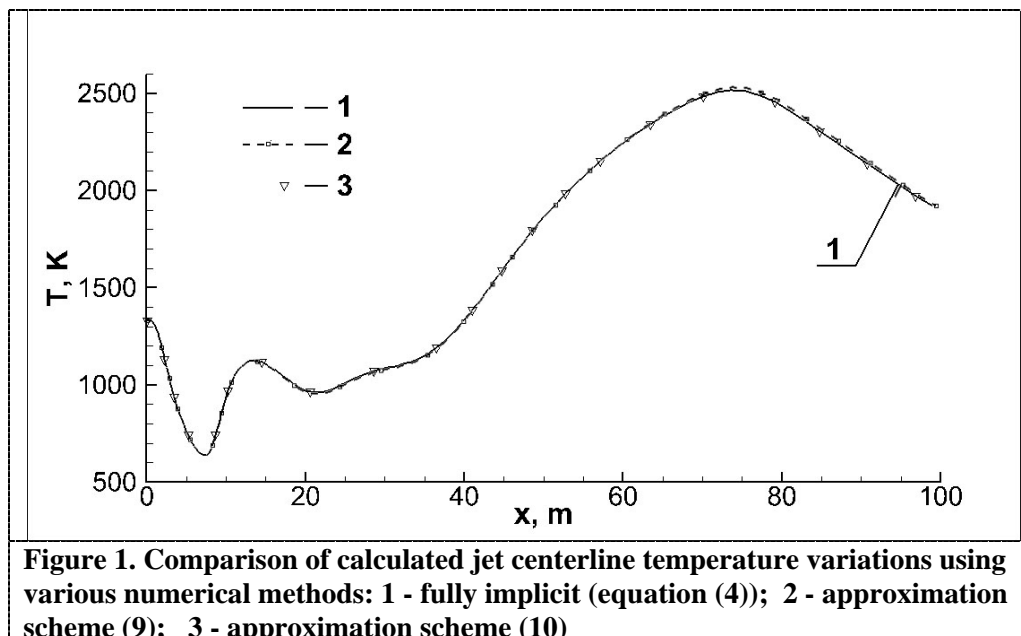


Figure 1. Comparison of calculated jet centerline temperature variations using various numerical methods: 1 - fully implicit (equation (4)); 2 - approximation scheme (9); 3 - approximation scheme (10)

Due to a great amount of H₂ и CO in the jet, chemical reaction with air causes powerful afterburning, which leads to a significant increase in temperature.

The calculation results for all three methods are in good agreement. Comparison of calculation time on a 120x60 mesh is presented in table 2.

Table 2. Comparison of calculation time on 120x60 mesh

Scheme	Fully implicit (equation (4))	Approximation scheme 1 (equation (9))	Approximation scheme 2 (equation (10))
Time, s	350	120	115

Obviously, the use of approximation schemes leads to a significant reduction in the calculation time. Approximation schemes 1 and 2 are not very different from each other.

4.2. Test 2

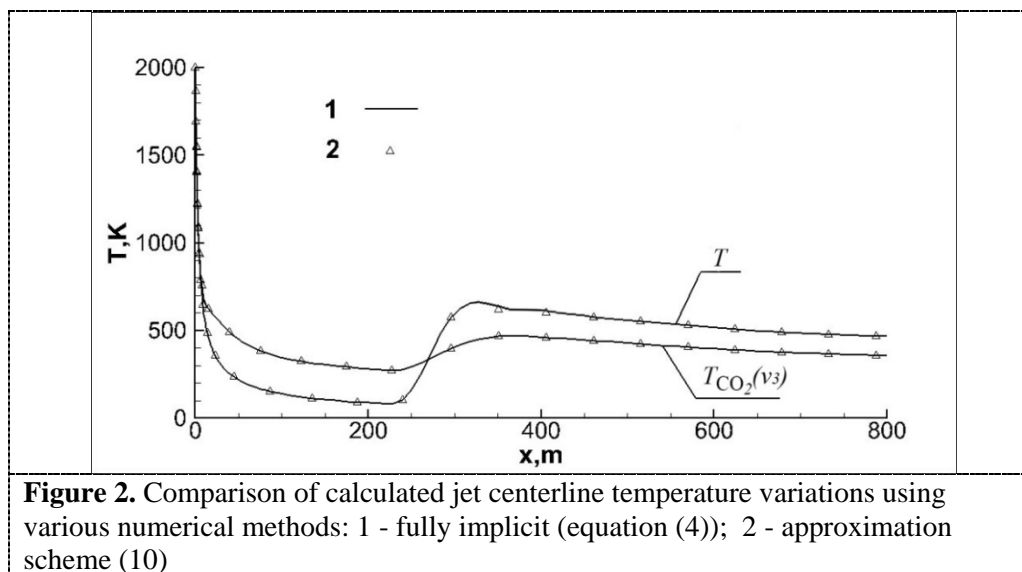
The jet of a model liquid engine was considered. The conditions at the nozzle exit (the temperature, velocity, pressure, mole fractions of gas components) and the nozzle radius chosen for the calculation are shown in the table 3.

Table 3. Conditions at the nozzle exit plane

T_a , K	U_a , M/c	R_a , M	P_a , ATM	H ₂	H ₂ O	CO	CO ₂	N ₂
2000	2500	0.5	0.3	0.05	0.4	0.05	0.15	0.35

The atmospheric conditions corresponded to an altitude of 80 km, the velocity of the external flow $U_e=2600$ m/s.

Figure 2 shows the results of calculating jet centerline temperature variations using various numerical methods. Shown: translational temperature T and vibrational temperature of the CO₂ asymmetric mode $T_{CO_2}(v_3)$.



The calculation results using the both schemes (fully implicit and approximation scheme (11)) coincide, both for translational and vibrational temperatures.

5. References

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