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ON A VARIANT OF THE METHOD OF CHARACTERISTICS FOR CALCULATING ONE-VELOCITY FLOWS OF A MULTICOMPONENT MIXTURE

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A variant of the method of characteristics for integration of equations defining one-velocity flows of a multicomponent mixture in the adiabatic approximation with the use of fixed grids is described.

Keywords: *one-velocity flow of a multicomponent mixture, hyperbolic systems, method of characteristics, numerical simulation.*

Introduction. For some time the method of characteristics was the main method used for calculating hyperbolic systems, among them gas-dynamics equations. Later, finite-difference methods found wide application, and the method of characteristics in its classical form was used much more rarely. Nevertheless, in a number of problems, correct boundary conditions can be set only with the use of this method; such conditions are used, in part, in calculations by finite-difference methods. The method of characteristics, due to its physical essence, allows one to perform calculations on a grid representing the structure of a flow most completely. This method is convenient for calculation of a rarefaction wave, construction of the lines of weak discontinuities, and determination of the sites of appearance of sudden shocks. However, the application of the method of characteristics is associated with a number of inconveniences, one of which is that the desired quantities are calculated at nodes of a characteristic grid that cannot be determined in advance. In practice it is desirable to know the distributions of parameters at fixed spatial points. In this case, it is necessary to use interpolation, which decreases the accuracy of calculations. Sometimes, calculations by the method of characteristics leads to a fairly inhomogeneous distribution of nodal points or to a large increase in the number of points on the characteristics. It should be noted that the method of characteristics can also be used, as in finite-difference schemes, in calculations on fixed grids without explicit separation of discontinuity surfaces. In this case, the classical method of characteristics described, e.g., in [1] should be changed. In the present work we describe one of such modified approaches developed for integration of one-velocity flows of a multicomponent mixture on a fixed spatial grid.

Model of a Heterogeneous Medium. We will consider an n-component mixture with the first m compressed fractions. The system of equations describing a heterogeneous-medium flow, in which the forces of interfraction interaction are taken into account, has the form (see [2]):

$$\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \mathbf{u}) = 0\,, \quad \rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\, \mathbf{u} \right] + \text{grad}\, p = \mathbf{F}\,,$$

$$\frac{\partial}{\partial t} \left[\rho \left(\varepsilon + \frac{1}{2} \, |\mathbf{u}|^2 \right) \right] + \text{div} \left[\rho \left(\varepsilon + \frac{1}{2} \, |\mathbf{u}|^2 + \frac{p}{\rho} \right) \mathbf{u} \right] = \mathbf{F} \cdot \mathbf{u}\,,$$

$$\frac{\partial \alpha_i \overset{0}{\rho}_i}{\partial t} + \text{div}\,(\alpha_i \overset{0}{\rho}_i \mathbf{u}) = \sum_{k=1}^{n(k \neq i)} J_{ik}\,, \tag{1}$$

$$\rho_i \left(\frac{\partial \varepsilon_i}{\partial t} + (\mathbf{u} \cdot \nabla)\, \varepsilon_i \right) + \frac{\alpha_i p}{\rho_i} \left[\sum_{k=1}^{n(k \neq i)} J_{ik} - \left(\frac{\partial \rho_i}{\partial t} + (\mathbf{u} \cdot \nabla)\, \rho_i \right) \right]$$

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$$= \sum_{k=1}^{n(k\neq i)} (R_{ik} + Q_{ik}) - \left(\varepsilon_i - \frac{1}{2}\,|\mathbf{u}|^2\right) \sum_{k=1}^{n(k\neq i)} J_{ik}\,, \quad i = 1, ..., m-1\,;$$

$$\frac{\partial \alpha_j}{\partial t} + \operatorname{div}(\alpha_j \mathbf{u}) = \frac{1}{\rho_j^0} \sum_{k=1}^{n(k\neq j)} J_{jk}\,, \quad j = m+1, ..., n\,.$$

The behavior of the compressed fractions is described by caloric equations of state, which have the form $\varepsilon_i = \varepsilon_i(p, \rho_i^0)$ for the ith fraction; therefore, the expression for the specific internal energy of the mixture

$$\varepsilon = \frac{1}{\rho} \sum_{i=1}^{n} \rho_i \varepsilon_i \tag{2}$$

can be written as

$$\varepsilon = \varepsilon\,(\rho, p, \alpha_1, \rho_1^0, ..., \alpha_{m-1}, \rho_{m-1}^0, \alpha_{m+1}, ..., \alpha_n)\,. \tag{3}$$

In the case where mass forces, phase and chemical transformations, and radiative heat transfer are absent in one-dimensional plane flows, the system of determining equations (1) is rearranged with the use of (3) to the form

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0\,, \quad \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0\,, \quad \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + \rho c^2 \frac{\partial u}{\partial x} = 0\,,$$

$$\frac{\partial \rho_i^0}{\partial t} + u \frac{\partial \rho_i^0}{\partial x} + \rho_i^0 G_i \frac{\partial u}{\partial x} = 0\,, \quad \frac{\partial \alpha_i}{\partial t} + u \frac{\partial \alpha_i}{\partial x} + \alpha_i\,(1 - G_i) \frac{\partial u}{\partial x} = 0\,, \quad i = 1, ..., m-1\,; \tag{4}$$

$$\frac{\partial \alpha_j}{\partial t} + u \frac{\partial \alpha_j}{\partial x} + \alpha_j \frac{\partial u}{\partial x} = 0\,, \quad j = m+1, ..., n\,.$$

The corresponding expressions for G_i and the velocity of sound c can be written as

$$G_i = \frac{1}{\rho_i^0} \left(\frac{\partial \varepsilon_i}{\partial \rho_i^0}\right)^{-1} \left(\frac{p}{\rho_i^0} - \rho c^2 \frac{\partial \varepsilon_i}{\partial p}\right), \tag{5}$$

$$c = \sqrt{\frac{\dfrac{p}{\rho} - \rho \dfrac{\partial \varepsilon}{\partial \rho} - \displaystyle\sum_{i=1}^{m-1} \left[\frac{p}{\rho_i^0} \frac{\partial \varepsilon}{\partial \rho_i^0} \left(\frac{\partial \varepsilon_i}{\partial \rho_i^0}\right)^{-1} + \alpha_i \frac{\partial \varepsilon}{\partial \alpha_i} \left(1 - p \left((\rho_i^0)^2 \frac{\partial \varepsilon_i}{\partial \rho_i^0}\right)^{-1}\right)\right] - \displaystyle\sum_{j=m+1}^{n} \alpha_j \frac{\partial \varepsilon}{\partial \alpha_j}}{\rho \left[\dfrac{\partial \varepsilon}{\partial p} + \displaystyle\sum_{i=1}^{m-1} \frac{\partial \varepsilon_i}{\partial p} \left(\frac{\partial \varepsilon_i}{\partial \rho_i^0}\right)^{-1} \left(\frac{\alpha_i}{\rho_i^0} \frac{\partial \varepsilon}{\partial \alpha_i} - \frac{\partial \varepsilon}{\partial \rho_i^0}\right)\right]}}\,.$$

In the case where the behavior of the mixture components is described with the use of the equation of state

$$\varepsilon_i = \frac{p - c_{*i}^2\,(\rho_i^0 - \rho_{*i})}{\rho_i^0\,(\gamma_i - 1)} = \frac{p B_i + b_i}{\rho_i^0} - d_i\,, \tag{6}$$

where $B_i = 1/(\gamma_i - 1)$, $d_i = c_{*i}^2 B_i$, and $b_i = d_i \rho_{*i}$, expression (2) takes the form

$$\varepsilon = \frac{1}{\rho}\left[pB_m + b_m + \sum_{i=1}^{m-1} \alpha_i \,(pB_{im} + b_{im} - d_{im}\rho_i^0) + \sum_{j=m+1}^{n} \alpha_j \rho_j^0 \varepsilon_j\right] - d_m \,. \tag{7}$$

Here, $B_{im} = B_i - B_m$, $b_{im} = b_i - b_m$, and $d_{im} = d_i - d_m$. The quantities G_i and c will be determined as

$$G_i = \frac{\rho c^2 B_i - p}{b_i + pB_i}\,, \quad c = \sqrt{\left\{b_m + p\left[1 + B_m - \sum_{i=1}^{m-1} \frac{\alpha_i\,(b_{im} + pB_{im})}{b_i + pB_i}\right]\right\} \Big/ \left\{\rho\left[B_m + \sum_{i=1}^{m-1} \frac{\alpha_i\,(b_m B_i - b_i B_m)}{b_i + pB_i}\right]\right\}}\ . \tag{8}$$

The characteristic equation of system (4) has only real eigenvalues: $u - c$, u, ..., $u + c$ (see [2]). The characteristic relations along the characteristic directions $dx/dt = u \pm c$ can be obtained from the equation

$$\begin{vmatrix}
\xi-u & -\rho & 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & -u\dfrac{d\rho}{dt}-\rho\dfrac{du}{dt} \\
0 & \xi-u & -\dfrac{1}{\rho} & 0 & 0 & \dots & 0 & 0 & 0 & \dots & -u\dfrac{du}{dt}-\dfrac{1}{\rho}\dfrac{dp}{dt} \\
0 & -\rho c^2 & \xi-u & 0 & 0 & \dots & 0 & 0 & 0 & \dots & -\rho c^2\dfrac{du}{dt}-u\dfrac{dp}{dt} \\
0 & -\rho_1^0 G_1 & 0 & \xi-u & 0 & \dots & 0 & 0 & 0 & \dots & -\rho_1^0 G_1\dfrac{du}{dt}-u\dfrac{d\rho_1^0}{dt} \\
0 & \alpha_1(G_1-1) & 0 & 0 & \xi-u & \dots & 0 & 0 & 0 & \dots & -\alpha_1(1+G_1)\dfrac{du}{dt}-u\dfrac{d\alpha_1}{dt} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & -\rho_{m-1}^0 G_{m-1} & 0 & 0 & 0 & \dots & \xi-u & 0 & 0 & \dots & -\rho_{m-1}^0 G_{m-1}\dfrac{du}{dt}-u\dfrac{d\rho_{m-1}^0}{dt} \\
0 & \alpha_{m-1}(G_{m-1}-1) & 0 & 0 & 0 & \dots & 0 & \xi-u & 0 & \dots & -\alpha_{m-1}(1+G_{m-1})\dfrac{du}{dt}-u\dfrac{d\alpha_{m-1}}{dt} \\
0 & -\alpha_{m+1} & 0 & 0 & 0 & \dots & 0 & 0 & \xi-u & \dots & -\alpha_{m+1}\dfrac{du}{dt}-u\dfrac{d\alpha_{m+1}}{dt} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & -\alpha_n & 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & -\alpha_n\dfrac{du}{dt}-u\dfrac{d\alpha_n}{dt}
\end{vmatrix} = 0,$$

where $\xi = dx/dt$. Calculation of the determinant gives expressions true at $dx/dt = u \pm c$:

$$dp \pm \rho c du = 0\,. \tag{9}$$

From system (4) follow equalities fulfilled along the trajectory characteristic $dx/dt = u$:

$$dp - c^2 d\rho = 0\,, \quad d\alpha_i - \frac{\alpha_i\,(1 - G_i)}{\rho}\, d\rho = 0\,, \quad d\rho_i - \frac{\rho_i}{\rho}\, d\rho = 0\,, \quad i = 1, ..., m-1\,; \tag{10}$$

$$d\rho - \frac{\rho}{\alpha_j}\, d\alpha_j = 0\,, \quad j = m+1, ..., n\,. \tag{11}$$

Integrating the latter expressions of (10) and expression (11), we obtain

$$\rho_i^0 = \rho_{i0}^0 \frac{\alpha_{i0}}{\alpha_i} \frac{\rho}{\rho_0}, \quad \alpha_j = \alpha_{j0} \frac{\rho}{\rho_0}. \tag{12}$$

Method of Characteristics for a Multicomponent Mixture. We will describe the procedure of solving the problem being considered with the use of the method of characteristics on a fixed spatial grid. For solving the problem it will suffice to determine the desired parameters at the node (x_k, t_{n+1}) by the known data at nodes of a finite-difference grid in the nth time layer. The problem will be solved using the following iteration procedure. It is assumed that, at the "zero" iteration ($s = 0$), the values of the desired functions at the point (x_k, t_{n+1}) are equal to the values of these functions at the point (x_k, t_n); therefore, the characteristic directions can be approximated by the expressions

$$x_k - x_{\rm L}^{(s)} = (u^{(s)} + c^{(s)})\,\Delta t\,, \quad x_k - x_{\rm C}^{(s)} = u^{(s)}\Delta t\,, \quad x_k - x_{\rm R}^{(s)} = (u^{(s)} - c^{(s)})\,\Delta t\,,$$

where $\Delta t = t_{n+1} - t_n$. From the latter equalities we determine the positions of the points of intersection of the characteristics with the straight line $t = t_n$ (see Fig. 1):

$$x_{\rm L}^{(s)} = x_k - (u^{(s)} + c^{(s)})\,\Delta t\,, \quad x_{\rm C}^{(s)} = x_k - u^{(s)}\Delta t\,, \quad x_{\rm R}^{(s)} = x_k - (u^{(s)} - c^{(s)})\,\Delta t\,. \tag{13}$$

The parameters p, u, ρ, and α_i at the points $x_{\rm L}$, $x_{\rm C}$, and $x_{\rm R}$ are determined by interpolation with the use of their known values at the nodes x_{k-1}, x_k, and x_{k+1}. The relations for the characteristic directions (9) and (10) are written in the finite-difference form

$$p^{(s+1)}(x_k, t_{n+1}) - p^{(s)}(x_{\rm L}, t_n) + \rho_{\rm L}^{(s)} c_{\rm L}^{(s)} (u^{(s+1)}(x_k, t_{n+1}) - u^{(s)}(x_{\rm L}, t_n)) = 0\,,$$

$$p^{(s+1)}(x_k, t_{n+1}) - p^{(s)}(x_{\rm R}, t_n) - \rho_{\rm R}^{(s)} c_{\rm R}^{(s)} (u^{(s+1)}(x_k, t_{n+1}) - u^{(s)}(x_{\rm R}, t_n)) = 0\,,$$

$$p^{(s+1)}(x_k, t_{n+1}) - p^{(s)}(x_{\rm C}, t_n) - (c_{\rm C}^{(s)})^2 (\rho^{(s+1)}(x_k, t_{n+1}) - \rho^{(s)}(x_{\rm C}, t_n)) = 0\,, \tag{14}$$

$$\alpha_i^{(s+1)}(x_k, t_{n+1}) - \alpha_i^{(s)}(x_{\rm C}, t_n) - \frac{\alpha_i^{(s)}(x_{\rm C}, t_n)\,(1 - G_{i{\rm C}}^{(s)})}{\rho^{(s)}(x_{\rm C}, t_n)} (\rho^{(s+1)}(x_k, t_{n+1}) - \rho^{(s)}(x_{\rm C}, t_n)) = 0\,.$$

Here, $G_{i{\rm C}}^{(s)} = \dfrac{\rho_{\rm C}^{(s)}(c_{\rm C}^{(s)})^2 B_i - p_{\rm C}^{(s)}}{b_i + p_{\rm C}^{(s)} B_i}$. Solving system (14) (at $s = 0$) for the variables $p^{(1)}$, $u^{(1)}$, $\rho^{(1)}$, and $\alpha_i^{(1)}$, we find the refined values of the desired functions at the point (x_k, t_{n+1}). At the first iteration, the true densities and the volume concentrations of the incompressible fractions are determined by formulas (12) from the expressions

$$(\rho_i^0)^{(s+1)}(x_k, t_{n+1}) = (\rho_i^0)^{(s)}(x_{\rm C}, t_n) \frac{\alpha_i^{(s)}(x_{\rm C}, t_n)}{\alpha_i^{(s+1)}(x_k, t_{n+1})} \frac{\rho^{(s+1)}(x_k, t_{n+1})}{\rho^{(s)}(x_{\rm C}, t_n)}\,,$$

$$\alpha_j^{(s+1)}(x_k, t_{n+1}) = \alpha_j^{(s)}(x_{\rm C}, t_n) \frac{\rho^{(s+1)}(x_k, t_{n+1})}{\rho^{(s)}(x_{\rm C}, t_n)}\,. \tag{15}$$

Then, by these data, from relations (13), we calculate the new coordinates $x_{\rm L}^{(1)}$, $x_{\rm C}^{(1)}$, and $x_{\rm R}^{(1)}$ that are used in turn for determining the values of $p^{(2)}$, $u^{(2)}$, $\rho^{(2)}$, $\alpha_i^{(2)}$, $(\rho_i^0)^2$, and $\alpha_j^{(2)}$ from (14)–(15) at $s = 1$. The iteration process described is continued as long as it converges.

To demonstrate the application of the above-described algorithm, we solved the problem on the breaking of an arbitrary shock in a gas-liquid mixture. The liquid fraction was assumed to be incompressible. The parameters of

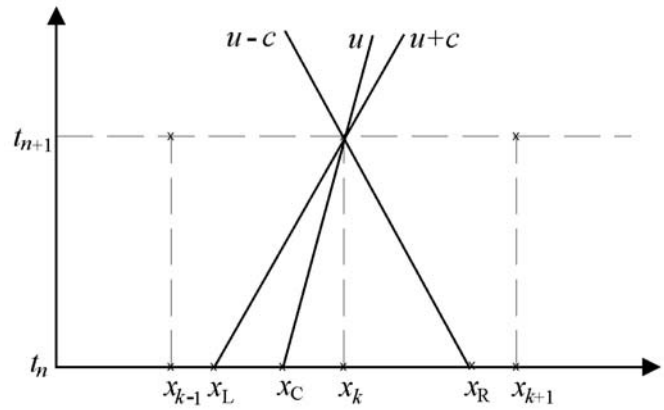

Fig. 1. Computational scheme.

the mixture before the breaking were as follows: at the left of the diaphragm ($x < 0$) $p_{0(1)}$ = 0.5 MPa, $u_{0(1)}$ = 0, $\alpha_{0(1)}$ = 0.9, $\rho^0_{10(1)}$ = 1.19 kg/m^3, $\gamma_{(1)}$ = 1.4, $\rho^0_{20(1)}$ = 1000 kg/m^3; at the right of the diaphragm ($x > 0$) $p_{0(2)}$ = 0.1 MPa, $u_{0(2)}$ = 0, $\alpha_{0(2)}$ = 0.9, $\rho^0_{10(2)}$ = 1.19 kg/m^3, $\gamma_{(2)}$ = 1.4, $\rho^0_{20(2)}$ = 1000 kg/m^3. At the instant of time t = 0, the diaphragm instantaneously moves to a great distance; in this case, the regime of flow with a shock wave moving to the right and a rarefaction wave moving to the left is realized.

Figure 2 presents results of calculations carried out by the method of characteristics at the instant of time t = 0.015 sec (points 1), which were compared with the exact solution of the Riemann problem (see [3]) (curves 2). In the calculations we used a uniform grid with a step h = 0.1 m. In the indicated figure, points 3 present results of solution of the Riemann problem at the instant of time t = 0.015 sec on the same computational grid but with the use of the finite-difference Courant–Isaacson–Riesz scheme (see [4]):

$$\frac{\mathbf{U}_i^{k+1} - \mathbf{U}_i^k}{\Delta t} + \mathbf{A}_i^k \frac{\mathbf{U}_{j+1/2}^k - \mathbf{U}_{i-1/2}^k}{\Delta x} = 0 ,$$

where

$$\mathbf{U}_{m+1/2}^k = \frac{1}{2} (\mathbf{U}_m^k + \mathbf{U}_{m+1}^k) + \frac{1}{2} \left\{ \Omega^{-1} [\text{sign} (\Lambda) \Omega] \right\}_m^k (\mathbf{U}_m^k - \mathbf{U}_{m+1}^k) , \quad m = i, i-1 .$$

Here,

$$\mathbf{U} = \begin{pmatrix} \rho \\ u \\ p \\ \alpha \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} u & \rho & 0 & 0 \\ 0 & u & 1/\rho & 0 \\ 0 & \rho c^2 & u & 0 \\ 0 & \alpha - 1 & 0 & u \end{pmatrix},$$

and the matrices Ω^{-1}, Λ, and Ω are determined in accordance with the formulas

$$\Omega = \begin{pmatrix} 0 & -\rho c & 1 & 0 \\ -c^2 & 0 & 1 & 0 \\ \dfrac{1}{\rho} & 0 & 0 & \dfrac{1}{1-\alpha} \\ 0 & \rho c & 1 & 0 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} u-c & 0 & 0 & 0 \\ 0 & u & 0 & 0 \\ 0 & 0 & u & 0 \\ 0 & 0 & 0 & u+c \end{pmatrix},$$

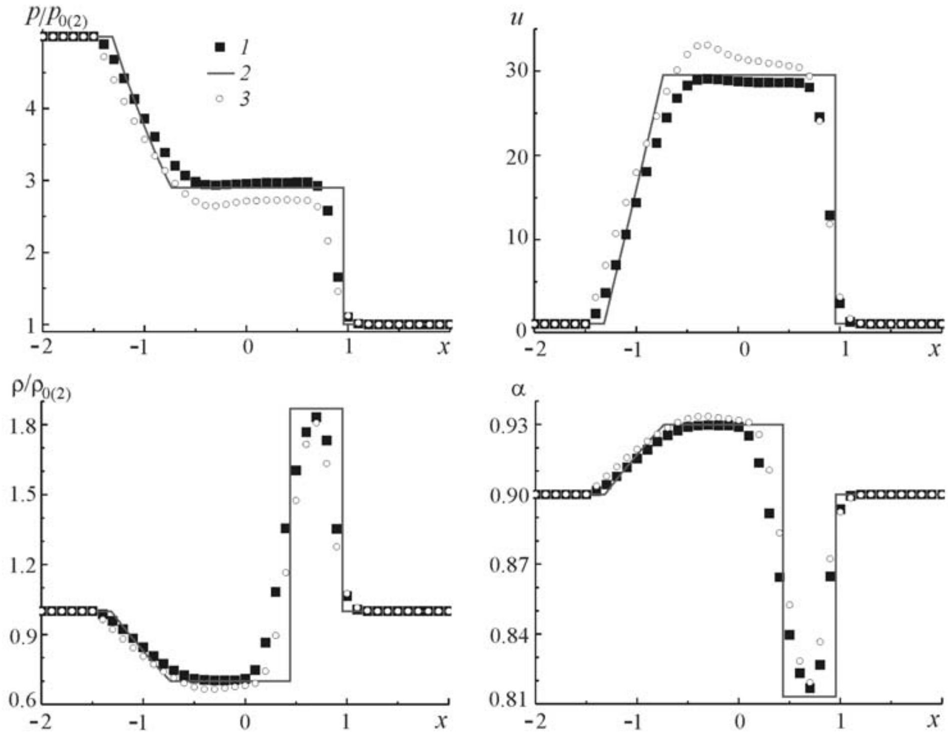

Fig. 2. Dependences of the parameters of the mixture on x in the case of breaking of a shock for t = 1.5 msec: 1) method of characteristics; 2) exact solution; 3) finite-difference Courant–Isaacson–Riesz scheme.

$$\Omega^{-1} = \begin{pmatrix} \frac{1}{2c^2} & -\frac{1}{c^2} & 0 & \frac{1}{2c^2} \\ -\frac{1}{2\rho c} & 0 & 0 & \frac{1}{2\rho c} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{\alpha - 1}{2\rho c^2} & \frac{1-\alpha}{\rho c^2} & 1-\alpha & \frac{\alpha - 1}{2\rho c^2} \end{pmatrix}.$$

It is seen from Fig. 2 that the method of characteristics gives more exact results as compared with the finite-difference scheme.

Conclusions. We described the method of characteristics for integration of one-dimensional equations defining a one-velocity flow of a multicomponent mixture in the adiabatic approximation on fixed spatial grids with continuous calculation of shocks. The approach considered can be directly extended to problems with several spatial variables. Moreover, this approach allows one to take into account the heat-conduction effect with the use of the hyperbolic model of a multicomponent heat-conducting mixture from [5].

NOTATION

c, adiabatic velocity of sound in a mixture; c_{*i}, constant of the equation of state; $\mathbf{F}$, density of the mass force; J_{ij}, intensity of transformation of the mass of a unit volume of the mixture from the ith fraction into the jth fraction; p, pressure; Q_{ij}, heat released in a unit time by a unit volume of the mixture due to the transformation of the ith fraction into the jth fraction; R_{ij}, heat released in a unit time by a unit volume of the mixture that is transferred from the jth fraction to the ith fraction by radiation; t, time; $\mathbf{u}(u)$, velocity vector (component); x, spatial variable; α_i, volume fraction; γ_i, constant of the equation of state; ε_i, specific internal energy; ρ, density of the mixture; ρ_i^0, real density of the ith fraction; $\rho_i = \alpha_i\rho_i^0$, reduced density of the ith component; ρ_{*i}, constant of the equation of state. Subscripts: 0, in a nondisturbed medium; (1), (2), for the parameters of the mixture at the "left" and at the "right" of the contact discontinuity; L (left), C (central), R (right), coordinates of the points of intersection of the characteristics $dx/dt = u + c$, $dx/dt = u$, and $dx/dt = u - c$ with the straight line $t = t_n$; k, number of a grid node; n, number of a time layer; (s), number of an iteration.

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