USING DIFFERENCE SCHEMES FROM THE GRID METHOD, WITH WEAK STABILITY LIMITATIONS FOR CALCULATIONS OF NONSTEADY NONISOTHERMAL FLOWS OF REAL GASES IN TUBES

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UDC 518.61:532.542

A numerical method is presented for the solution of a system of equations for nonsteady nonisothermal motion of a real gas in tubes, this procedure based on the application of the so-called asymmetrical explicit difference schemes of the grid method, which is characterized by weak stability limitations.

When we consider the physically important factors associated with the presence of heat transfer with respect to an external medium, as well as the real thermodynamic properties of a gas in the solution of practical problems dealing with the calculation of one-dimensional gas flows in tubes, we find it necessary to consider the general equations of gas dynamics, in which the compressibility factor $Z_0(P, T)$, the specific capacity $c_p(P, T)$, etc., can be specified analytically or in tabular form.

The latter circumstance, as well as the complexity of the very system of partial differential equations leads to the practical impossibility of achieving exact analytical solutions, in connection with which it becomes necessary to employ numerical methods involving the use of computer calculations. In this case, to apply the grid method we must transform the original equations into a system of evolutionary-type quasi-linear equations whose right-hand members contain the second derivative of the square of the pressure with respect to the three-dimensional variable. The form of the equation derived in this case proved to be exceedingly convenient for application of the explicit difference schemes, both of the classical type [1, 2], and also – particularly – of their modifications, based on the utilization of asymmetrical difference equations. These schemes were effective in the numerical solution of a rather cumbersome system of equations for the nonsteady nonisothermal motion of a real gas in tubes. Exhibiting the advantages of explicit difference schemes – economy and simple logic – the difference schemes considered below are characterized by a weak stability limitation which permits a rather large time interval τ, thus offering a real possibility of realizing these schemes with a computer. At the same time, the modifications of the explicit schemes, with use of the asymmetrical difference equations, provide rather high (approximately of the order of $O(h^2)$) degrees of accuracy for the resulting numerical solutions and we have a computation algorithm which is analogous to the scheme of a two-point running count. In this sense, the use of explicit difference schemes and the cited modifications of the grid method for the solution of the specific equations under consideration proved to be more preferable than the implicit schemes associated with the pivot method or with iterations [6].

1). The nonsteady nonisothermal flow of real gases in long conduits is described [1] by the following system of equations:

$$\Delta \frac{\partial P}{\partial t} = \frac{1}{2a}\left[\frac{1}{2bG}\frac{\partial^2 P^2}{\partial x^2} + G\frac{\partial}{\partial x}(Z_0 T)\right] - \left(Z_0 + T\frac{\partial Z_0}{\partial T}\right)\left[\frac{1}{a}G\frac{\partial T}{\partial x} + bc\frac{G^3 T^3 Z_0}{P^2}\frac{\partial Z_0}{\partial T} - n(T^* - T)\right]; \quad (1)$$

$$\Delta \frac{\partial T}{\partial t} = \frac{T}{P}\left\{\frac{1}{2a}\left[\frac{1}{2bG}\frac{\partial^2 P^2}{\partial x^2} + G\frac{\partial}{\partial x}(Z_0 T)\right]\left(Z_0 + T\frac{\partial Z_0}{\partial T}\right) m + Z_0\left[\frac{1}{a}G\frac{\partial T}{\partial x} + bc\frac{G^3 T^3 Z_0}{P^2}\frac{\partial Z_0}{\partial T} - n(T^* - T)\right]\left(\frac{P}{Z_0}\frac{\partial Z_0}{\partial P} - 1\right)\right\}; \quad (2)$$

Computer Center, Academy of Sciences of the USSR, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 16, No. 2, pp. 308-315, February, 1969. Original article submitted April 29, 1968.

$$\frac{\partial P^2}{\partial x} = -2bZ_0TG^2, \qquad (3)$$

where

$$\Delta \equiv 1 - \frac{P}{Z_0}\frac{\partial Z_0}{\partial P} - \frac{m}{Z_0}\left(Z_0 + T\frac{\partial T_0}{\partial T}\right)^2 \neq 0; \quad Z_0 = Z_0(P, T);$$
$$a = \frac{f}{R}; \quad b = \frac{\lambda R}{2gDf^2}; \quad c = \frac{AR^2}{c_p f}; \quad m = \frac{AR}{c_p}; \quad n = \frac{K\pi DR}{c_p f}. \qquad (4)$$

A finite-difference scheme of the explicit classical four-point scheme was used in earlier references [1, 2] to solve Eqs. (1)-(3). The existence of a term with the second derivative $\partial^2P^2/\partial x^2$ in the first of the equations in (1)-(3) imposes a limitation of the form $\tau = O(h^2)$ on the intervals h and τ, from the conditions of stability, and this limitation with respect to Eq. (1), in linear approximation, can be written as follows:

$$\frac{\tau}{h^2} \leqslant bd \min\left(\Delta_{i,k}\frac{G_{i,k}}{P_{i,k}}\right).$$

Since this inequality is not a rigorous condition of stability for the sytem of equations (1)-(3), it permits us tentatively to evaluate the order of magnitude for the step τ which ensures the stability of the (k + 1)-th time layer being calculated. The final magnitude of the interval τ is corrected and subsequently determined in the process of the practical calculation of system (1)-(3). As shown by calculation, inequality (4) imposes no rigorous limitations on the time step τ, with the exception of the cases in which G becomes small or vanishes at some point of the integration interval. If G is small, condition (4) results in such a small interval τ that to realize the explicit difference scheme on a computer would require extensive machine time. When G is equal to zero, the use of this scheme may result in an unstable calculation process. We see from Eq. (3) that these features (the smallness of G or the vanishing of the latter) are governed by the constancy of the pressure distribution in the specified integration interval or by the fact that the pressure varies only slightly. Similar features are encountered, for example, in the problem of filling or emptying a gas conduit; in the problem of stabilizing temperature and pressure in a gas conduit that has been shut down [5], etc. We note that when P(x, t) = const for $0 \leq x \leq L$ and for a fixed instant t, we obviously have

$$G(x, t) = \frac{\partial G}{\partial x} = 0, \quad \frac{\partial P}{\partial x} = \frac{\partial^2 P^2}{\partial x^2} = 0.$$

The original equations in the form of (1) and (2) exhibit the following feature in this case: the term $1/G\ \partial^2P^2/\partial x^2$ yields an indeterminacy of the 0/0 type. Expanding this indeterminacy, with consideration of Eq. (3), we find

$$\frac{1}{G}\frac{\partial^2 P^2}{\partial x^2} = -2b\frac{1}{G}\frac{\partial}{\partial x}(G^2TZ_0) = -2b\left[2\frac{\partial G}{\partial x}Z_0T + G\frac{\partial}{\partial x}(Z_0T)\right] = 0.$$

To improve the stability of the finite-difference equations approximating the original system, in these cases we can construct explicit difference schemes based on the utilization of asymmetrical difference equations. These schemes exhibit less rigorous limitations on stability, as compared to the classical explicit difference scheme, thus making it possible substantially to reduce the expenditure of machine time in the numerical computer realization of the corresponding boundary problems. With a difference approximation of the differential operators, in this case the second derivative with respect to x in the given differential equations is approximated nonsymmetrically. As a result, the portion of the second derivative with some weight σ is extended forward, i.e., to the (k + 1)-th layer being calculated. A similar method has been described in [3] for linear equations of the parabolic type; a similar scheme was used in the numerical solution of a nonlinear equation for the case of isothermal gas motion [4]. Here the method associated with the use of asymmetrical explicit difference schemes is extended to the case of a system of quasilinear differential equations (1)-(3).

2). Denoting

$$A = \frac{G}{2a}\frac{\partial}{\partial x}(Z_0T) - \left(Z_0 + T\frac{\partial Z_0}{\partial T}\right)\left[\frac{1}{a}G\frac{\partial T}{\partial x} + bc\frac{G^3T^3Z_0}{P^2}\frac{\partial Z_0}{\partial T} - n(T^* - T)\right],$$

$$B = \frac{G}{2a} \frac{\partial}{\partial x} (Z_0 T) \left(Z_0 + T \frac{\partial Z_0}{\partial T} \right) m$$

$$+ Z_0 \left[\frac{1}{a} G \frac{\partial T}{\partial x} + bc \frac{G^3 T^3 Z_0}{P^2} \frac{\partial Z_0}{\partial T} - n (T^* - T) \right] \left(\frac{P}{Z_0} \frac{\partial Z_0}{\partial P} - 1 \right),$$

from (1) and (2) we obtain

$$\frac{\partial P}{\partial t} = \frac{\frac{1}{4abG} \frac{\partial^2 P^2}{\partial x^2} + A}{\Lambda}, \tag{5}$$

$$\frac{\partial T}{\partial t} = \frac{T}{P} \frac{\frac{A_1(P,T)}{4abG} \frac{\partial^2 P^2}{\partial x^2} + B}{\Delta}, \text{ where } A_1(P, T) = \left(Z_0 + T \frac{\partial Z_0}{\partial T} \right) m. \tag{6}$$

We will apply the following difference approximation for the derivatives in Eqs. (5) and (6):

$$\left(\frac{\partial P}{\partial t} \right)_{i,k} = \frac{P_{i,k+1} - P_{i,k}}{\tau} + O(\tau), \tag{7}$$

$$\left(\frac{\partial^2 P^2}{\partial x^2} \right)_{i,k} = \frac{1}{h} \left[\left(\frac{\partial P^2}{\partial x} \right)_{i+\frac{1}{2},k} - \left(\frac{\partial P^2}{\partial x} \right)_{i-\frac{1}{2},k} \right] + O(h^2). \tag{8}$$

Using the representation of the derivative $\partial P^2/\partial x$ in the form of a Taylor series, we obviously find

$$\left(\frac{\partial P^2}{\partial x} \right)_{i-\frac{1}{2},k} = \left(\frac{\partial P^2}{\partial x} \right)_{i-\frac{1}{2},k+1} - \tau \frac{\partial^2 P^2 \left(x_{i-\frac{1}{2}}, t_k + \theta\tau \right)}{\partial x \partial t}, \quad 0 \leqslant \theta \leqslant 1. \tag{9}$$

Having introduced the parameter σ, from (7) and (8) we find the following representation for the second derivative of the square of the pressure:

$$\left(\frac{\partial^2 P^2}{\partial x^2} \right)_{i,k} = \frac{\sigma}{h^2} \left[\left(\frac{\partial P^2}{\partial x} \right)_{i+\frac{1}{2},k} - \left(\frac{\partial P^2}{\partial x} \right)_{i-\frac{1}{2},k+1} \right]$$

$$- \frac{1-\sigma}{h} \left[\left(\frac{\partial P^2}{\partial x} \right)_{i+\frac{1}{2},k} - \left(\frac{\partial P^2}{\partial x} \right)_{i-\frac{1}{2},k} \right] + \frac{\sigma\tau}{h} \frac{\partial^2 P^2 \left(x_{i-\frac{1}{2}}, t_k + \theta\tau \right)}{\partial x \partial t} + O(h^2). \tag{10}$$

Using the difference approximation for the first derivatives of the form

$$\left(\frac{\partial P^2}{\partial x} \right)_{i-\frac{1}{2},k+1} = \frac{P^2_{i,k+1} - P^2_{i-1,k+1}}{h} + O(h^2),$$

$$\left(\frac{\partial P^2}{\partial x} \right)_{i+\frac{1}{2},k} = \frac{P^2_{i+1,k} - P^2_{i,k}}{h} + O(h^2),$$

we have

$$\left(\frac{\partial^2 P^2}{\partial x^2} \right)_{i,k} = \frac{\sigma}{h^2} (P^2_{i-1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i+1,k}) + \frac{1-\sigma}{h} (P^2_{i-1,k} - 2P^2_{i,k} + P^2_{i+1,k}) + O\left(\sigma \frac{\tau}{h} + h^2 \right). \tag{11}$$

Considering (7) and (11), we obtain the following difference approximation of (5) and (6):

$$\Delta_{i,k} \frac{P_{i,k+1} - P_{i,k}}{\tau} = \frac{1}{4abG_{i,k}} \left[\frac{\sigma}{h^2} (P^2_{i-1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i+1,k}) \right.$$

$$\left. + \frac{1-\sigma}{h^2} \left(P^2_{i-1,k} - 2P^2_{i,k} + P^2_{i+1,k} \right) \right] + A_{i,k} + \Delta_{i,k} R_{i,k}, \tag{12}$$

$$\Delta_{i,k} \frac{T_{i,k+1} - T_{i,k}}{\tau} = \frac{T_{i,k}}{P_{i,k}} \left\{ \frac{(A_1)_{i,k}}{4abG_{i,k}} \left[\frac{\sigma}{h^2} (P^2_{i-1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i+1,k}) \right. \right.$$

$$\left. \left. + \frac{1-\sigma}{h^2} (P^2_{i-1,k} - 2P^2_{i,k} + P^2_{i+1,k}) \right] + B_{i,k} \right\} + \Delta_{i,k} R_{i,k}, \tag{13}$$

where

$$R_{i,k} = O\left(\sigma \frac{\tau}{h} + h^2 + \tau\right), \quad 0 \leqslant \sigma \leqslant 1. \tag{14}$$

Equations (12) and (13) are calculated from left to right, i.e., beginning from the boundary conditions specified at the left-hand end of the integration interval ($x = l_1$). The difference approximation for the same equations can be derived in similar manner in the form

$$\frac{P_{i,k+1}-P_{i,k}}{\tau} = \left\{\frac{1}{4abG_{i,k}}\left[\frac{\sigma}{h^2}(P^2_{i+1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i-1,k}) + \frac{1-\sigma}{h^2}(P^2_{i+1,k} - 2P^2_{i,k} + P^2_{i-1,k})\right] + A_{i,k}\right\}\Big/\Delta_{i,k} + R_{i,k}, \tag{15}$$

$$\frac{T_{i,k+1}-T_{i,k}}{\tau} = \frac{T_{i,k}}{P_{i,k}}\left\{\frac{(A_1)_{i,k}}{4abG_{i,k}}\left[\frac{\sigma}{h^2}(P^2_{i+1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i-1,k}) + \frac{1-\sigma}{h^2}(P^2_{i+1,k} - 2P^2_{i,k} + P^2_{i-1,k})\right] + B_{i,k}\right\}\Big/\Delta_{i,k} + R_{i,k}. \tag{16}$$

Equations (15) and (16) are calculated from right to left. We note that when $\sigma = 0$ both forms of the approximations (12), (13), (15), and (16) lead to the identical classical explicit difference scheme. For $\sigma = 1$ we find another limit case. Multiplying (12) and (13) by h^2 and neglecting the small quantity $h^2 R_{i,k}$, we derive the following formulas for the calculation of P and T at the nodes of the approximation grid:

$$P_{i,k+1} = \frac{2ab\Delta_{i,k}}{\sigma}\left[-\delta G_{i,k} + \sqrt{(\delta G_{i,k})^2 + \frac{\sigma}{ab\Delta_{i,k}}C^*}\right], \tag{17}$$

$$T_{i,k+1} = T_{i,k} + \delta\frac{T_{i,k}}{P_{i,k}}\left\{\frac{(A_1)_{i,k}}{4abG_{i,k}} \times\left[\sigma(P^2_{i-1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i+1,k}) + (1-\sigma)(P^2_{i-1,k} - 2P^2_{i,k} + P^2_{i+1,k})\right] + h^2 B_{i,k}\right\}\Big/\Delta_{i,k},$$

where

$$C^* = \delta P_{i,k}G_{i,k} + \frac{1}{\Delta_{i,k}}\left\{\frac{1}{4ab}\left[\sigma(P^2_{i-1,k+1} - P^2_{i,k} + P^2_{i+1,k}) + (1-\sigma)(P^2_{i-1,k} - 2P^2_{i,k} + P^2_{i+1,k})\right] + h^2 A_{i,k}G_{i,k}\right\},$$

$$\delta = \frac{h^2}{\tau}. \tag{18}$$

Analogously, on the basis of (15) and (16) we can derive the working formulas for T and P, calculated from right to left:

$$P_{i,k+1} = \frac{2ab\Delta_{i,k}}{\sigma}\left[-\delta G_{i,k} + \sqrt{(\delta G_{i,k})^2 + \frac{\sigma}{ab\Delta_{i,k}}D}\right], \tag{19}$$

$$T_{i,k+1} = T_{i,k} + \delta\frac{T_{i,k}}{P_{i,k}}\left\{\frac{(A_1)_{i,k}}{4abG_{i,k}}\left[\sigma(P^2_{i+1,k+1} - P^2_{i,k+1} - P^2_{i,k} + P^2_{i-1,k}) + (1-\sigma)(P^2_{i+1,k} - 2P^2_{i,k} + P^2_{i-1,k})\right] + h^2 B_{i,k}\right\}\Big/\Delta_{i,k}, \tag{20}$$

where

$$D = \delta P_{i,k}G_{i,k} + \frac{1}{\Delta_{i,k}}\left\{\frac{1}{4ab}\left[\sigma(P^2_{i+1,k+1} - P^2_{i,k} + P^2_{i-1,k}) + (1-\sigma)(P^2_{i+1,k} - 2P^2_{i,k} + P^2_{i-1,k})\right]\right\}.$$

After we have calculated P and T from (17) and (18) or from (19) and (20), we determine G from (3).

It should be pointed out that in the special case in which T = const, Z_0 = const, and m = 0, system (1)-(3) degenerates into the familiar system of equations for the nonsteady isothermal motion of an ideal gas

$$\frac{\partial G}{\partial x} = -a^*\frac{\partial P}{\partial t}, \tag{21}$$

TABLE 1. Comparison of the Theoretical Data in the Use of Various Explicit Difference Schemes

$\bar{x}$	$\bar{t}$	I ($\tau/h^2=1$)			II ($\tau/h^2=16$)			III ($\tau/h^2=32$)		
		P	T	G	P	T	G	P	T	G
0	10	1,201	1,679	0,682	1,201	1,679	0,660	1,201	1,679	0,644
0,2		1,167	1,457	0,775	1,169	1,450	0,763	1,170	1,446	0,752
0,4		1,129	1,424	0,824	1,132	1,424	0,811	1,134	1,424	0,801
0,6		1,085	1,411	0,868	1,089	1,411	0,860	1,092	1,412	0,855
0,8		1,034	1,397	0,927	1,039	1,398	0,928	1,043	1,398	0,925
1,0		0,972	1,369	1,000	0,977	1,382	1,000	0,981	1,382	1,000
0	20	1,201	1,679	0,788	1,201	1,679	0,781	1,201	1,679	0,773
0,2		1,158	1,535	0,816	1,158	1,529	0,815	1,159	1,524	0,812
0,4		1,111	1,440	0,884	1,112	1,436	0,887	1,113	1,434	0,884
0,6		1,060	1,417	0,921	1,061	1,416	0,923	1,062	1,416	0,921
0,8		1,002	1,406	0,954	1,002	1,404	0,961	1,004	1,004	0,959
1,0		0,936	1,377	1,000	0,935	1,393	1,000	0,937	1,392	1,000
0	30	1,201	1,679	0,847	1,201	1,679	0,845	1,201	1,679	0,840
0,2		1,151	1,568	0,853	1,151	1,567	0,854	1,152	1,566	0,850
0,4		1,101	1,479	0,891	1,101	1,474	0,879	1,102	1,472	0,896
0,6		1,046	1,430	0,936	1,045	1,428	0,943	1,046	1,427	0,942
0,8		0,985	1,414	0,966	0,983	1,413	0,973	0,984	1,413	0,973
1,0		0,916	1,387	1,000	0,913	1,404	1,000	0,914	1,403	1,000
0	40	1,201	1,679	0,887	1,201	1,679	0,888	1,201	1,679	0,884
0,2		1,146	1,576	0,889	1,146	1,576	0,891	1,146	1,576	0,888
0,4		1,092	1,505	0,904	1,091	1,504	0,909	1,092	1,503	0,907
0,6		1,034	1,452	0,937	1,033	1,450	0,944	1,034	1,448	0,944
0,8		0,971	1,424	0,969	0,968	1,423	0,977	0,969	1,422	0,977
1,0		0,899	1,395	1,000	0,896	1,411	1,000	0,897	1,411	1,000

Note: I correspond to the explicit classical scheme of the grid method; II and III correspond to a scheme involving the use of asymmetrical difference equations (17) and (18) when $\sigma = 1$. The results giving in the table have been rounded off to the third significant figure. When $\bar{t} = 0$ for $\bar{x} = 0, \ldots, 1.0$ P = 1.201; T = 1.443; G = 0.

$$\frac{\partial P}{\partial x} = -b^* \frac{G^2}{P},$$

where

$$a^* = \text{const}, \quad b^* = \text{const},$$

or to the system equivalent to the above:

$$\frac{\partial P}{\partial t} = \frac{1}{4a^*b^*G} \frac{\partial^2 P^2}{\partial x^2}, \qquad (22)$$

$$\frac{\partial P^2}{\partial x} = -2b^*G^2.$$

From (17)-(20), as a special case we can derive the finite-difference formulas for the calculation of the parameters of isothermal gas flow. As we see from (14), the error in the approximation of the differential equations (1)-(3) by the difference equations (17)-(20) is of the order of $O(h)$ when $\sigma \neq 0$. When $\sigma = 0$ the magnitude of the error will be at a minimum, while it reaches a maximum for $\sigma = 1$. Here the errors in the difference formulas (17)-(20) are opposite in sign. This circumstance serves as the basis for the various modifications of the grid method involving the use of the above-considered difference schemes which are characterized by a higher degree of accuracy for the resulting numerical solutions. In particular, these include the so-called intermittent method and the method of the arithmetic mean. The intermittent method involves the alternating use of Eqs. (17)-(20). For example, the odd time layers are calculated from (17) and (18), while the even layers are calculated from (19) and (20).

In using the method of the arithmetic mean we find that the calculation of the unknown quantities P and T for each time layer is accomplished as follows: formulas (17) and (18) are used to calculate the equations from left to right; formulas (19) and (20) are used to calculate the equations from right to left. As the final values for the unknowns at each layer we use the arithmetic mean of the corresponding results from two calculations. As shown for the linear parabolic equations [3], with an increase in the parameter σ the corresponding stability conditions for the difference schemes under consideration become less rigorous. When

$\sigma = 1$ the analogous difference scheme for one linear parabolic equation is absolutely stable. As demonstrated by numerical calculations (Table 1), in the case of the system of equations (1)-(3) the stability limitations in the use of the above-considered difference schemes exhibit the same tendency toward weakening with a change in the quantity σ as in the linear case.

Table 1 shows selected results of calculations with respect to the conditions cited in [2], with the use of difference schemes of the explicit classical scheme of the grid method, and with the use of asymmetrical difference equations for $\sigma = 1$. As we can see from a comparison of the results, for various relationships between the step h and τ the maximum divergence with respect to P and T does not exceed approximately 1% (at the point $x = 1.0$), and with respect to $G \sim 4\%$. The difference schemes considered here thus yield virtually identical results; however, schemes involving the use of asymmetrical difference equations permit us to use a substantially greater time step τ (greater by a factor of approximately 30 for the conditions of the specific example). The noted advantages of these schemes make their application extremely effective for gas and thermodynamic calculations of main gas conduits, where the expenditure of machine time in the design of a single gas-conduit segment becomes substantial when using conventional explicit schemes.

NOTATION

P	is the pressure;
T, T*	are, respectively, the gas and soil temperatures;
G	is the weight flow rate;
λ	is the coefficient of hydraulic resistance;
D, f	are, respectively, the diameter and area of the tube cross section;
Z_0, R	are, respectively, the coefficient of compressibility and the gas constant;
A	is the heat equivalent of work;
K	is the coefficient of heat transfer from the gas to the soil;
t	is the time;
x	is the coordinate along the axis of the gas conduit;
τ, h	are, respectively, the time step and the coordinate.

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