

STIFFNESS PROBLEM IN MODELING WAVE FLOWS OF HETEROGENEOUS MEDIA WITH A THREE-TEMPERATURE SCHEME OF INTERPHASE HEAT AND MASS TRANSFER

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UDC 518.517.0

The numerical modeling of wave flows of heterogeneous media with a three-temperature scheme of interphase heat and mass transfer involves the problem of equation stiffness. A discrete model of improved stability was developed to describe these processes. Test calculations of the interaction of a shock wave with a bounded layer of a mixture of a gas and droplets assuming a discrete model over a wide range of initial data showed that the stability conditions do not depend on the rate of interphase interaction (C-stability).

Introduction. Designing new technologies and methods of protecting from intense shock-wave, thermal, and vibrational actions using heterogeneous media requires in-depth study of the motion of mixtures undergoing phase transitions with allowance for the temperature and velocity nonequilibrium of phases. Usually, these problems can be solved only numerically on the basis of discrete models (difference schemes). Problems of numerically modeling wave flows of heterogeneous media were studied in [1, 2] and others. Schemes for calculating gas wave flows with solid particles and droplets were developed in [3, 4]. Mathematical modeling of wave flows of heterogeneous media is characterized by a greater (e.g., than in gas-dynamic problems) number of equations of motion and closure relations, which calls for more powerful computers. Therefore, development of economical methods for numerical solutions of this class of problems seems especially important.

As shown in [5–7], in calculating gas filtration in a porous medium and wave flows of a mixture of a gas and solid particles, in which interphase interactions (friction and heat exchange) are rather intense, the step in time must be significantly restricted. It should be noted that the Courant criterion (see e.g., [6]) imposes less rigorous constraints on the admissible step of integration.

A similar problem arises in numerical integration of ordinary differential equations of some types by classical methods [8], where the time scales of some components of the solution vector differ significantly. For this type of ordinary differential equations, the term of “stiffness” was introduced and implicit methods were shown to be more effective for their numerical solution.

In the above sense, a wide class of problems of the motion of heterogeneous media is described by stiff partial differential equations, e.g., in cases where the characteristic times of equalization of phase velocities and temperatures are significantly smaller than the time of perturbation propagation at the distance equal to the characteristic grid size. Discrete models with explicit approximation of space derivatives and implicit allowance for source terms [5–7] enables a severalfold increase in the stability factor. For some classes of flows, the stability factor can be increased by an order of magnitude and more, which is supported by numerous calculations for various flows of mixtures of a gas and solid particles. An important property of such discrete models is C-stability (the stability conditions for a scheme over a wide range of initial data are determined by the Courant criterion and are independent of the rate of interphase interactions). This property is especially important in solving multidimensional problems, where the point of calculation domain at which the solution becomes unstable is not known beforehand. Thus, for example,

Mozhaiskii Military Space-Engineering University, St. Petersburg 197082. Translated from *Prikladnaya Mekhanika i Tekhnicheskaya Fizika*, Vol. 43, No. 2, pp. 136–141, March–April, 2002. Original article submitted May 28, 2001; revision submitted August 23, 2001.

in calculations using a scheme that is not C-stable, instability can be manifested after several time steps due to a sharp increase in interphase-transfer rate, thus necessitating repeated calculations using smaller time steps.

The stiffness problem also arises in numerical modeling of wave flows of a gas-droplet mixture with phase transitions, in particular using a three-temperature scheme of interphase heat and mass transfer [1], in which the temperature field in the vicinity of a droplet is characterized by the temperatures of the gas T_1 , the droplet T_2 , and the interface T_Σ . The heat fluxes per unit volume from the drop surface to the gas of the mixture and the fluid are given by the expression

$$Q_{\Sigma i} = 1.5(\alpha_2/r^2)\text{Nu}_i\lambda_i(T_\Sigma - T_i), \quad i = 1, 2. \quad (1)$$

Here α_i are the volume fractions of the phases, r is the droplet radius, λ_i is the thermal conductivity of the i th phase, and Nu_i is the Nusselt number ($\text{Nu}_2 = 10$ [1], and the value of Nu_1 is obtained experimentally [9]). The mass-transfer rate per unit volume J_{12} is determined from the relation

$$J_{12}l(p_v) = Q_{\Sigma 1} + Q_{\Sigma 2}, \quad (2)$$

where $l(p_v)$ is the heat of evaporation and p_v is the partial vapor pressure.

In calculations using a three-temperature scheme, the mechanism of the instability development can be explained as follows. Let the droplets evaporate ($J_{12} < 0$) at a certain time step τ , which brings about an increase in vapor density ρ_{1v} and partial pressure p_v . On the assumption of phase equilibrium at the interface $T_\Sigma = T_s(p_v)$, the average temperature at it also increases. Therefore, if the value of τ is not small, then, according to (1) and (2), evaporation gives way to condensation, after which the parameter-fluctuation amplitudes become unbounded.

This paper is an attempt to construct a C-stable noniterative discrete model for the wave motion of a gas-droplet mixture allowing for the difference in phase velocity using a three-temperature scheme of heat and mass transfer and the stiffness concept.

Governing Equations. Let us consider a two-phase disperse mixture of droplets with a two-component carrier phase (inert gas and vapor). Let us adopt the well-known assumptions used in the mechanics of collisionless monodisperse mixtures [1]: the droplet sizes are many times larger than the molecular-kinetic sizes and many times smaller than the distances over which the averaged mixture parameters change significantly; the mixture is monodisperse, the chaotic and internal motion (rotation and deformation) of disperse particles can be neglected; no processes of collision, grinding, coalescence, and formation of new droplets take place; the viscosity and thermal conductivity of the phases are manifested only in the processes of interphase interaction; the condensed phase is undeformed; the components of the carrier phase (inert gas and vapor) do not enter chemical reactions among each other and satisfy the additivity conditions; gravitational forces are neglected. With allowance for the earlier assumptions and inertia effects for the flow around the droplets, the equations of conservation of mass, momentum, and energy of the phases and the mixture are written as

$$\begin{aligned} \frac{\partial \rho_{1g}}{\partial t} + \nabla \cdot (\rho_{1g} \mathbf{v}_1) &= 0, & \frac{\partial \rho_{1v}}{\partial t} + \nabla \cdot (\rho_{1v} \mathbf{v}_1) &= -J_{12}, \\ \frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \mathbf{v}_2) &= J_{12}, & \frac{\partial \rho_2 r}{\partial t} + \nabla \cdot (\rho_2 r \mathbf{v}_2) &= \frac{4}{3} r J_{12}, \\ \frac{\partial \rho_1 \mathbf{v}_1}{\partial t} + \nabla \cdot (\rho_1 \mathbf{v}_1 \mathbf{v}_1) &= -\beta_1 \nabla p + J_{12} \left(\beta_1 \mathbf{w}_{12} - \beta_2 \frac{\alpha_2}{2} \frac{\rho_1}{\rho_2} \mathbf{w}_{12} - \mathbf{v}_1 \right) - \alpha_1 \beta_2 \mathbf{F}_\mu, \\ \frac{\partial \rho_2 \mathbf{v}_2}{\partial t} + \nabla \cdot (\rho_2 \mathbf{v}_2 \mathbf{v}_2) &= -(1 - \beta_1) \nabla p + J_{12} \left((1 - \beta_1) \mathbf{w}_{12} + \beta_2 \frac{\alpha_2}{2} \frac{\rho_1}{\rho_2} \mathbf{w}_{12} + \mathbf{v}_2 \right) + \alpha_1 \beta_2 \mathbf{F}_\mu, \\ \frac{\partial \rho_2 u_2}{\partial t} + \nabla \cdot (\rho_2 u_2 \mathbf{v}_2) &= Q_{\Sigma 2} + J_{12} u_{2\Sigma}, \\ \frac{\partial}{\partial t} (\rho_1 E_1 + \rho_2 E_2) + \nabla \cdot (\rho_1 E_1 \mathbf{v}_1 + \rho_2 E_2 \mathbf{v}_2) + \nabla \cdot (p(\alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2)) &= 0, \\ \beta_1 &= \frac{\alpha_1 (2 + \chi_m \rho_1^0 / \rho_2^0)}{2 + \chi_m (\alpha_2 + \alpha_1 \rho_1^0 / \rho_2^0)}, & \beta_2 &= \frac{2}{2 + \chi_m (\alpha_2 + \alpha_1 \rho_1^0 / \rho_2^0)}. \end{aligned} \quad (3)$$

Here the subscripts ‘‘g,’’ and ‘‘v’’ denote the parameters of the inert and vapor components of the gas, respectively, the subscript Σ denotes the parameters of the surface phase (Σ -phase), E_i and u_i are the specific total energy

and internal energy of the i th phase, p is the pressure, \mathbf{F}_μ is the rate of the viscous force interphase interaction, and χ_m is coefficient that allows for the effect of non-uniqueness and non-sphericity of the droplets on the force of attached masses.

The viscous friction force exerted by the gas on the condensed phase in a unit volume is specified as in [1]:

$$\mathbf{F}_\mu = 0.75 \frac{\alpha_2}{r} C_\mu \frac{\rho_1^0 w_{12}}{2} \frac{\mathbf{w}_{12}}{w_{12}}, \quad C_\mu = C_\mu(\text{Re}_{12}, \alpha_2), \quad \text{Re}_{12} = \frac{2r \rho_1^0 w_{12}}{\mu_1}, \quad \mathbf{w}_{12} = \mathbf{v}_1 - \mathbf{v}_2.$$

Here Re_{12} is the Reynolds number of the relative phase motion and C_μ is the empirically obtained [10, 11] friction coefficient.

The system of conservation equations (3) is closed by the equations of state of calorifically perfect gas components:

$$\begin{aligned} p_g &= \rho_{1g}^0 R_{1g} T_1, & p_v &= \rho_{1v}^0 R_{1v} T_1, & p &= p_g + p_v, \\ \rho_1^0 &= \rho_{1g}^0 + \rho_{1v}^0, & k_{1g} &= \rho_{1g}^0 / \rho_1^0, & k_{1v} &= \rho_{1v}^0 / \rho_1^0 \quad (k_{1g} + k_{1v} = 1), \\ u_1 &= k_{1g} u_{1g} + k_{1v} u_{1v}, & \lambda_1 &= \lambda_1(k_{1g}, T_1), & i_g &= c_g(T_1 - T^*) + i_g^*, & i_v &= c_v(T_1 - T^*) + i_v^*. \end{aligned} \quad (4)$$

Here p_g is the partial pressure of the inert gas, R_{1g} and R_{1v} are the constants of the gas components, ρ_{1g}^0 and ρ_{1v}^0 , k_{1g} and k_{1v} , and u_{1g} and u_{1v} are the true densities, mass fractions, and internal energies of a unit mass of the components, respectively, c_g and c_v are the heat capacities of the inert gas and vapor at constant pressure, and i_g is the enthalpy of the gas component; the superscript “*” denotes fixed parameters. The enthalpy of the vapor component i_v is related to the enthalpy of the condensed phase i_l by the normalization condition

$$i_v^* - i_l^* = l(p_v^*) + (c_l - c_v)(T_s(p_v^*) - T^*),$$

where c_l is the heat capacity of the fluid.

Discrete Model. In developing a discrete model, we use splitting into physical processes [12], in which all interphase interactions are calculated only in the first stage. As preliminary analysis shows, for the “rapid” components of the solution, implicit allowance for the source terms is required.

In accordance with (3), the local change in vapor density is determined by the phase-transition rate in a unit volume:

$$(\tilde{\rho}_{1v} - \rho_{1v}^k) / \tau = -\tilde{J}_{12} \quad (5)$$

(k is the time step number; tilde denotes the values calculated in the first stage). Using the heat- and mass-transfer relations (1) and (2), Eq. (5) can be written as

$$\frac{\tilde{\rho}_{1v} - \rho_{1v}^k}{\tau} = -\frac{(\alpha_{s1}^k + \alpha_{s2}^k)}{l(p_v^k)} \tilde{T}_s + \frac{\alpha_{s1}^k}{l(p_v^k)} T_1^k + \frac{\alpha_{s2}^k}{l(p_v^k)} T_2^k, \quad \alpha_{si} = 1.5 \frac{\alpha_2}{r^2} \text{Nu}_i \lambda_i, \quad (6)$$

where α_{si} are the coefficients of heat transfer between the Σ -phase and the i th phase in a unit volume.

For noniterative calculation of the vapor density in (6), the function $T_s(p_v)$ can be linearized as is done in [6] for interphase friction:

$$\tilde{T}_s = T_s^k + \left(\frac{\partial T_s}{\partial p_v} \right)^k (\tilde{p}_v - p_v^k). \quad (7)$$

The temperature on the saturation line is usually represented as a polynomial $T_s^k = \sum_{j=0}^n c_j (p_v^k)^j$, hence

$$\tilde{T}_s = c'_0 + \tilde{p}_v \sum_{j=1}^n c'_j (p_v^k)^{j-1}, \quad c'_0 = c_0 - \sum_{j=1}^n (j-1) c_j (p_v^k)^j, \quad c'_j = j c_j.$$

Finally, with allowance for the equation of state for the vapor component (4), the relation for the preliminary value of the vapor density (6) is written as

$$\tilde{\rho}_{1v} = \left(\rho_{1v}^k - \tau \frac{\alpha_{s1}^k + \alpha_{s2}^k}{l(p_v^k)} c'_0 + \tau \left(\frac{\alpha_{s1}^k}{l(p_v^k)} T_1^k + \frac{\alpha_{s2}^k}{l(p_v^k)} T_2^k \right) \right) / \left(1 + \tau \frac{\alpha_{s1}^k + \alpha_{s2}^k}{l(p_v^k)} \frac{R_v T_1^k}{\alpha_1^k} \sum_{j=1}^n c'_j (p_v^k)^{j-1} \right).$$

Using the implicit method of calculating interphase interactions for other equations of system (3), in the first step of calculation, we have

$$\tilde{\rho}_{1v} = \left(\rho_{1v}^k - \tau \frac{\alpha_{s1}^k + \alpha_{s2}^k}{l(p_v^k)} c'_0 + \tau \left(\frac{\alpha_{s1}^k}{l(p_v^k)} T_1^k + \frac{\alpha_{s2}^k}{l(p_v^k)} T_2^k \right) \right) / \left(1 + \tau \frac{\alpha_{s1}^k + \alpha_{s2}^k}{l(p_v^k)} \frac{R_v T_1^k}{\alpha_1^k} \sum_{j=1}^n c'_j (p_v^k)^{j-1} \right).$$

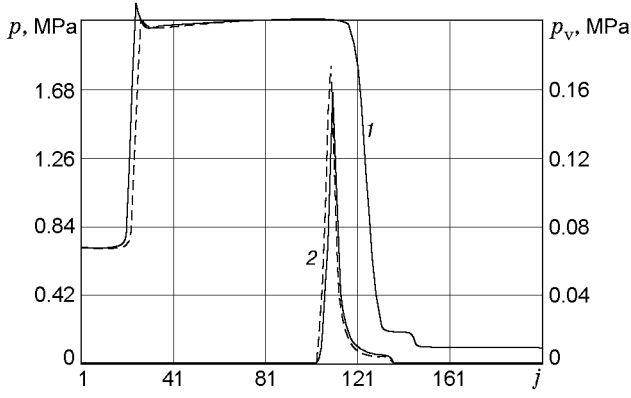


Fig. 1

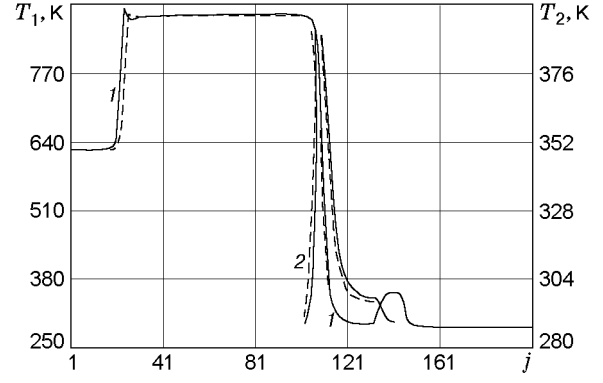


Fig. 2

Fig. 1. Profiles of gas pressure (curves 1) and partial vapor pressure (curves 2): solid curves refer to calculations using the scheme (8), (9) and dashed curves refer to calculations using the scheme of [3].

Fig. 2. Temperature profiles for the gas (curves 1) and droplets (curves 2): solid curves refer to calculations using the scheme (8), (9) and dashed curves refer to calculations using the scheme of [3].

$$\begin{aligned}
(\tilde{\rho}_{1v} - \rho_{1v}^k)/\tau &= -\tilde{J}_{12}, & (\tilde{\rho}_2 - \rho_2^k)/\tau &= \tilde{J}_{12}, \\
\frac{\tilde{\rho}_2 \tilde{r} - \rho_2^k r^k}{\tau} &= \frac{4}{3} \tilde{J}_{12} \tilde{r} \quad \text{for } \tilde{J}_{12} < 0, & \frac{\tilde{\rho}_2 \tilde{r} - \rho_2^k r^k}{\tau} &= \frac{4}{3} \tilde{J}_{12} r^k \quad \text{for } \tilde{J}_{12} > 0, \\
\frac{\tilde{\rho}_1 \tilde{\mathbf{v}}_1 - \rho_1^k \mathbf{v}_1^k}{\tau} &= -\beta_1^k \nabla p^k + J_{12}^k \left(\beta_1^k \mathbf{w}_{12}^k - \beta_2^k \frac{\alpha_2^k}{2} \frac{\rho_1^k}{\rho_2^k} \mathbf{w}_{12}^k - \mathbf{v}_1^k \right) - \alpha_1^k \beta_2^k \tilde{\mathbf{F}}_\mu (\tilde{\mathbf{v}}_1 - \mathbf{v}_2^k), \\
\frac{\tilde{\rho}_2 \tilde{\mathbf{v}}_2 - \rho_2^k \mathbf{v}_2^k}{\tau} &= -(1 - \beta_1^k) \nabla p^k + J_{12}^k \left((1 - \beta_1^k) \mathbf{w}_{12}^k + \beta_2^k \frac{\alpha_2^k}{2} \frac{\rho_1^k}{\rho_2^k} \mathbf{w}_{12}^k + \mathbf{v}_2^k \right) + \alpha_1^k \beta_2^k \tilde{\mathbf{F}}_\mu (\tilde{\mathbf{v}}_1 - \mathbf{v}_2^k), \\
(\tilde{\rho}_2 \tilde{u}_2 - \rho_2^k u_2^k)/\tau &= \tilde{Q}_{\Sigma 2} (\tilde{T}_s - \tilde{T}_2) + \tilde{J}_{12} u_{2\Sigma}^k, & \tilde{E}_2 &= \tilde{u}_2 + (\tilde{\mathbf{v}}_2)^2/2, \\
\frac{(\tilde{\rho}_1 \tilde{E}_1 + 0.5 \tilde{\rho}_2 \tilde{\mathbf{v}}_2) - (\rho_1^k E_1^k + 0.5 \rho_2^k \mathbf{v}_2^k)}{\tau} &= \tilde{Q}_{\Sigma 1} (\tilde{T}_s - \tilde{T}_1) - \tilde{J}_{12} (l(p_v^k) + u_{2\Sigma}^k) - \nabla \cdot (p^k (\alpha_1^k \mathbf{v}_1^k + \alpha_2^k \mathbf{v}_2^k)), \\
\tilde{T}_2 &= (\tilde{u}_2 - u_2^*)/c_2 + T^*, & \tilde{T}_1 &= (\tilde{E}_1 - \tilde{\mathbf{v}}_1^2/2 - k_{1v} u_{1v}^* - k_{1g} u_{1g}^*)/c_{1v} + T_1^*.
\end{aligned} \tag{8}$$

Here c_{1v} is the heat capacity of the two-component gas in a constant volume.

In the second stage, the final values of the desired parameters are obtained with allowance for the fluxes of masses, pulses, and energies of the phases through the cell boundaries (using a standard procedure), taking into account their directions [12]:

$$\begin{aligned}
(\rho_{1g}^{k+1} - \rho_{1g}^k)/\tau + \nabla \cdot (\rho_{1g}^k \tilde{\mathbf{v}}_1) &= 0, & (\rho_{1v}^{k+1} - \rho_{1v}^k)/\tau + \nabla \cdot (\rho_{1g}^k \tilde{\mathbf{v}}_1) &= 0, \\
(\rho_2^{k+1} - \rho_2^k)/\tau + \nabla \cdot (\tilde{\rho}_2 \tilde{\mathbf{v}}_2) &= 0, & (\rho_2^{k+1} r^{k+1} - \rho_2^k r^k)/\tau + \nabla \cdot (\tilde{\rho}_2 \tilde{r} \tilde{\mathbf{v}}_2) &= 0, \\
(\rho_1^{k+1} \mathbf{v}_1^{k+1} - \rho_1^k \mathbf{v}_1^k)/\tau + \nabla \cdot (\tilde{\rho}_1 \tilde{\mathbf{v}}_1 \tilde{\mathbf{v}}_1) &= 0, & (\rho_2^{k+1} \mathbf{v}_2^{k+1} - \rho_2^k \mathbf{v}_2^k)/\tau + \nabla \cdot (\tilde{\rho}_2 \tilde{\mathbf{v}}_2 \tilde{\mathbf{v}}_2) &= 0, \\
(\rho_2^{k+1} u_2^{k+1} - \rho_2^k u_2^k)/\tau + \nabla \cdot (\tilde{\rho}_2 \tilde{u}_2 \tilde{\mathbf{v}}_2) &= 0, \\
(\rho_1^{k+1} E_1^{k+1} + \rho_2^{k+1} E_2^{k+1} - (\tilde{\rho}_1 \tilde{E}_1 + \tilde{\rho}_2 \tilde{E}_2))/\tau + \nabla \cdot (\tilde{\rho}_1 \tilde{E}_1 \tilde{\mathbf{v}}_1 + \tilde{\rho}_2 \tilde{E}_2 \tilde{\mathbf{v}}_2) &= 0.
\end{aligned} \tag{9}$$

Test Calculations. The proposed scheme was tested by solving the one-dimensional problem of interaction of a rectangular shock wave with a bounded layer of a mixture of air and water droplets which was in phase equilibrium at the initial time.

The initial data are as follows: incident wave Mach number $1 \leq M_0 \leq 4$, initial volume fraction of water droplets in the layer $\alpha_{20} \leq 0.1$, the initial droplet radius $r_0 \geq 10 \mu\text{m}$, $T_{10} = T_{20} = T_{s0} = 293 \text{ K}$, and $p_0 = 10^5 \text{ Pa}$. The properties of water and water vapor are taken from the tabulated data of [13] and approximated by fifth-degree polynomials.

The calculations were carried out using a through-calculation scheme. In the case of $\rho_2 < 10^{-6} \text{ kg/m}^3$ and $r < 10^{-9} \text{ m}$, calculations of interphase interactions which did not influence significantly accuracy were eliminated from the algorithm to reduce the volume of computations. The uniform grid included 200 cells of size $h \leq 0.01 \text{ m}$. Cell Nos. 81–120 contained a gas suspension layer with the parameters indicated above. At the left boundary, boundary conditions were specified as the parameters of the incident shock wave, and at the right boundary, the specified boundary conditions were “mild” (extrapolation of parameters inside the calculation domain). The time step was chosen from the condition

$$\tau = \text{Ku} h / \max_j |v_{1,j} + a_{1,j}| \quad (\text{Ku} \leq 1), \quad (10)$$

where Ku is the Courant number, a_1 is the velocity of sound in the gas, and j is the cell number.

As test calculations showed, within the range studied, the proposed discrete model (8), (9) is C-stable. The stability factor depends only on the Courant criterion (10) and is independent of the rate of interphase interactions. The Courant number for which the calculation is stable for the noniterative model (8), (9), is an order of magnitude larger than the Courant number in the calculation scheme with explicit allowance for the interphase transfer [3]. For example, for $M_0 = 2.5$, $\alpha_{20} = 0.1$, $r_0 = 10 \mu\text{m}$, and $h = 0.01 \text{ m}$, the scheme [3] is unstable in the range $0.07 \leq \text{Ku}_2 \leq 1$. As analysis of the calculations shows, the instability is caused by significant fluctuations of the interface temperature T_s at the front of the shock wave entering the layer and leads to an unbounded increase of the solution. For $\text{Ku}_2 \leq 0.07$, a solution is possible with bounded oscillations of large amplitude, which practically vanish when $\text{Ku}_2 \simeq 0.02$. The proposed discrete model (8), (9) provides for stable calculations for $\text{Ku}_1 = 1$.

Figures 1 and 2 show the results of calculations using the scheme (8), (9) and the explicit scheme [3] at $\text{Ku}_1 = 1$, $\text{Ku}_2 = 0.02$, and $t = 0.004 \text{ sec}$. Decrease in the time step determined by Courant number $\text{Ku}_1 \leq 0.2$ leads to the practical coincidence of the both solutions.

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