NUMERICAL SOLUTION OF PHASE-CHANGE PROBLEMS

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Abstract-A three-time level implicit scheme, which is unconditionally stable and convergent, is employed for the numerical solution of phase-change problems, on the basis of an analytical approach consisting in the approximation of the latent heat effect by a large heat capacity over a small temperature range. Since the temperature dependent coefficients in the resulting parabolic equations are evaluated at the intermediate time level, the complication of solving a set of nonlinear algebraic equations at each time step is avoided. The numerical results thus obtained are satisfactorily compared with the available analytical solutions.

NOMENCLATURE

- c, specific heat $[J/kgK]$;
- $C = c\rho$, volumetric heat capacity $[J/m^3K]$;
- **e**,
f, local order of accuracy $\lceil K/s \rceil$;
- surface temperature $\lceil {^{\circ}C} \rceil$;
- H, enthalpy per unit volume $[J/m^3]$;
- k, thermal conductivity $\lceil W/mK \rceil$;

$$
K, \qquad \text{thermal conductivity integral [W/m];}
$$

slab thickness [m];

L, slab thickness $[m]$;
 $0(\Delta x^2)$, the remainder in Taylor series expansion and of the order (Δx^2) ;

 t_{\star} temperature: solution of the heat conduction equations $\lceil {^{\circ}C} \rceil$;

7: temperature: solution ofthe numerical equations $[^{\circ}C]$;

x, y, z, position coordinates [m].

Greek letters

 y_x , difference operator:

 $\gamma_x T_i = T_{i-\frac{1}{2}} - T_{i-\frac{1}{2}};$

 δ . Dirac "function":

- Δx , grid spacing in the x direction $\lceil m \rceil$;
- Δt , temperature semi-interval across t_f $\lceil K \rceil$:

Δτ. time step [s]:

- step function; $\eta,$
- heat of phase change per unit volume λ . $[J/m^3]$;

$$
(\mu \gamma)_t, \quad \text{difference operator:} \\ (\mu \gamma)_t T^h = \frac{\gamma_t T^{h + \frac{1}{2}} + \gamma_t T^{h - \frac{1}{2}}}{2}
$$

$$
=\frac{T^{h+1}-T^{h-1}}{2};
$$

Ĕ. phase front position $[m]$;

density $\left[\frac{kg}{m^3}\right]$; ρ ,

time $[s]$; τ.

initial temperature distribution $\lceil {^{\circ}C} \rceil$. φ .

Subscripts

a. surface;

- f , phase change;
- $i,$ lattice parameter in a one-dimensional grid: $x = i\Delta x$;
- reference : r.
- $\overline{0}$. initial:
- 1, solid region;
- 2, liquid region.

Superscripts

- h, time level: $\tau = h\Delta \tau$;
- equivalent;
- approximated.

INTRODUCTlON

A LARGE number of current applications of engineering interest involve solution of the equation describing heat conduction with a change of phase. However, while many important theoretical results are available about existence uniqueness, and properties of classical solutions (see e.g. $[7, 8]$), the literature surveys $[2, 3, 19, 21]$ reveal that most actual analytical solutions deal only with the one-dimensional geometry and very special boundary conditions and cannot thus be extended to many practical problems.

Numerical methods have also been proposed by several authors (see $\lceil 10, 21 \rceil$) but, especially in the multidimensional case, their applicability is limited by their great complexity. Therefore it can be inferred that the conventional mathematical description, considering an interface surface which moves either into the solid region (melting) or into the liquid region (freezing) in accordance with the relative magnitudes of the temperature gradients on either side of it, does not yield to a general mathematical formulation which combines good accuracy with computational ease.

Fortunately another model is possible which has a sound theoretical basis and leads to a much more compact and convenient analytical formulation.

Most phase-change processes involve substances which, like the foodstuffs or the metal alloys, are not pure and, therefore, the latent heat effect can be expressed by a finite temperature dependent heat capacity, since it occurs over a temperature range [4,23].

This feature suggests that the true latent heat effect in pure substances can be approximated by a large heat capacity over a small temperature range. Such an intuitive approach, proposed in [1. 241, has been employed in recent years for

numerical calculations in $[6, 9, 11, 22]$, while a rigorous analysis, based on the concept of "generalized (weak) solution" and including a convergence proof, has been given in [12, 13, 15,201. Nevertheless this procedure has not been used as much as its simplicity would suggest. This is undoubtedly due to the difficulties involved in the solution of the resulting heat conduction equation which has critically temperature dependent coefficients.

The intent of the present work is to show how a three-time level difference method, which has been recently proposed for the solution of heat conduction problems when the thermophysical properties depend on temperature $[4, 5]$, can be advantageously applied also to the solution of melting and freezing problems, provided that they are formulated as previously outlined.

FORMULATION OF THE PROBLEM

Usually a problem with a phase transition of a substance from one state to another, in the one-dimensional case under boundary conditions of the first kind, is mathematically formulated as follows [18]

$$
C_1(t)\frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left[k_1(t)\frac{\partial t}{\partial x}\right]; \qquad 0 < x < \xi(\tau),
$$
\n
$$
\tau > 0; \qquad (1)
$$

$$
t_1(x,0) = \varphi_1(x) \leq t_f; \qquad 0 < x < \xi(0); \tag{2}
$$

$$
t_1(0, \tau) = f_1(\tau) < t_f; \qquad \tau > 0,\tag{3}
$$

where subscript 1 refers to the "solid" region, and :

$$
C_2(t)\frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left[k_2(t)\frac{\partial t}{\partial x}\right];
$$

$$
\xi(\tau) < x < L, \quad \tau > 0; \quad (4)
$$

$$
t_2(x, 0) = \varphi_2(x) \ge t_f; \qquad \xi(0) < x < L; \qquad (5)
$$

$$
t_2(L, \tau) = f_2(\tau) > t_f; \quad \tau > 0 \tag{6}
$$

where subscript 2 refers to the "liquid" region.* $\overline{}$

^{*} Each of (3) and (6) can be replaced by a condition of prescribed x-derivate on $x = 0$, $x = L$ respectively. In (1)-(6) one assumes $0 < \xi(0) < L$; trivial modifications are needed in this scheme for the cases $\xi(0) = 0$ or $\xi(0) = L$.

(7)

On the interface it is

an d

$$
k_2(t)\frac{\partial t_2}{\partial x} - k_1(t)\frac{\partial t_1}{\partial x} = \lambda \frac{\mathrm{d}\xi}{\mathrm{d}\tau}
$$
 (8)

where λ is the heat of phase change per unit volume.

 $t_1[\xi(\tau), \tau] = t_2[\xi(\tau), \tau] = t_f$

However, based on a physical approach, a different mathematical model can be tried. Boundary condition (8) , in fact, stems from the "jump" of magnitude λ which the enthalpy per unit volume H undergoes at the temperature of the phase transition t_f . Therefore, from the enthalpy definition

$$
H(t) = \int_{t_r}^t C(t) dt + \lambda \eta(t - t_f);
$$

\n
$$
\eta(u) = \begin{cases} 1, & u \ge 0 \\ 0, & u < 0 \end{cases}
$$
 (9)

where $t_r < t_f$ is arbitrarily chosen, an "equivalent" heat capacity per unit volume $\tilde{C}(t)$ can also be defined $[6, 15, 20, 22]$

$$
\tilde{C}(t) = \frac{dH(t)}{dt} = C(t) + \lambda \delta(t - t_f);
$$
\n
$$
C(t) = \begin{cases} C_1(t), & t < t_f \\ C_2(t), & t > t_f \end{cases} \tag{10}
$$

where $\delta(t - t_f)$ is the Dirac-function.

Substituting in equations (1) and (4) the following expression is derived

$$
\tilde{C}(t)\frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left[k(t)\frac{\partial t}{\partial x}\right];
$$
\n
$$
k(t) = \begin{cases} k_1(t), & t < t_f \\ k_2(t), & t > t_f \end{cases}
$$
\n(11)

It can be shown that every sufficiently smooth solution of (11), such that the regions $t > t_f$, $t < t_f$ are separated by a unique continuously differentiable curve $x = \xi(\tau)$, verifies condition (8). In fact, let us consider the integrals I_1 and I_2 of the left and right members of equation (11) in a small layer $(\xi - \varepsilon \leq x \leq \xi + \varepsilon)$ symmetrical with respect to the interface and then let us take the limits as $\varepsilon \to 0$. The following relationships are obtained

$$
\lim_{\varepsilon \to 0} I_{1} = \lim_{\varepsilon \to 0} \int_{\varepsilon - \varepsilon}^{\varepsilon + \varepsilon} \tilde{C}(t) \frac{\partial t}{\partial \tau} dx
$$
\n
$$
= \lim_{\varepsilon \to 0} \left[\int_{\varepsilon - \varepsilon}^{\varepsilon + \varepsilon} C(t) \frac{\partial t}{\partial \tau} dx + \int_{t(\xi - \varepsilon, \tau)}^{t(\xi + \varepsilon, \tau)} \lambda \delta(t - t_{f}) \frac{\partial x}{\partial \tau} dt \right] = \lambda \frac{d\xi}{d\tau} \qquad (12)
$$
\n
$$
\lim_{\varepsilon \to 0} I_{2} = \lim_{\varepsilon \to 0} \int_{\xi - \varepsilon}^{\xi + \varepsilon} \frac{\partial}{\partial x} \left[k(t) \frac{\partial t}{\partial x} \right] dx =
$$
\n
$$
\lim_{\varepsilon \to 0} \left[k(t) \frac{\partial t}{\partial x} \right]_{x = \xi + \varepsilon} - k(t) \frac{\partial t}{\partial x} \Big|_{x = \xi - \varepsilon} \qquad (13)
$$

Since $I_1 = I_2$, condition (8) can be immediately derived. Therefore, if a numerical solution is tried, instead of starting from the conjugated problems (1) and (4) coupled through condition (8), a single equation (11) can be considered. Actually this step is not a straightforward one: equation (11), in fact, involves a delta-function in the definition of $\tilde{C}(t)$ and must be regarded thus as a "generalized" formulation for problem (1) , (4) and (8) , to be dealt with on the basis of the theory of distributions. However, due to the practical intent of this work, only the theoretical results which are needed to further proceed with a meaningful numerical solution will be mentioned :

1. Under suitable assumptions (unessential for practical purposes) on the data and the coefficients, there exists a generalized solution to the problem (11) , (2) , (3) , (5) and (6) [†] which is unique and, by means of elementary calculations, can be shown to coincide with the classical solution to the original problem (1) - (8) whenever the latter exists.

2. Such a solution can be obtained as the limit of a uniformly convergent sequence of classical solutions to approximating problems, deduced by smoothing the coefficients in equation (11) following a few general rules:

(a) The delta-function in the definition of $\bar{C}(t)$ must be replaced by a deltaform function $\delta(t - t_f, \Delta t)$ which assumes large but finite values in the semi-interval Δt across t_f where it is different from zero. Consequently a smoothed heat capacity $C^*(t)$ can be defined

$$
C^*(t) = \begin{cases} C_1(t), & t < t_f - \Delta t \\ C_2(t), & t > t_f + \Delta t \end{cases} \tag{14}
$$

and

$$
\int_{t_f-\Delta t}^{t_f+\Delta t} C^*(t) dt = \lambda + \int_{t_f-\Delta t}^{t_f} C_1(t) dt + \int_{t_f}^{t_f+\Delta t} C_2(t) dt
$$
\n(15)

which retains the enthalpy variations.

(b) Similarly a smoothed thermal conductivity $k^*(t)$ has to be introduced, subjected to the conditions

$$
k^*(t) = \begin{cases} k_1(t), & t < t_f - \Delta t \\ k_2(t), & t > t_f + \Delta t \end{cases} \tag{16}
$$

 $\hat{\tau}$ A generalized solution to the problem (11), (2), (3), (5) and (6) in the rectangle: $0 \le x \le L$, $0 \le t \le \theta$ is every measurable function $t(x, t)$ satisfying the integral identity θ 1.

$$
\int_{0}^{L} \int_{0}^{L} \left\{ H[u(x, \tau)] \frac{\partial}{\partial \tau} F(x, \tau) + K[u(x, \tau)] \frac{\partial^{2}}{\partial x^{2}} F(x, \tau) \right\} dx dt
$$

+
$$
\int_{0}^{L} H[\varphi(x)] F(x, 0) dx + \int_{0}^{0} \left\{ K[f_{1}(\tau)] \frac{\partial}{\partial x} F(x, \tau) \Big|_{x=0} \right\} dt = K[f_{2}(\tau)] \frac{\partial}{\partial x} F(x, \tau) \Big|_{x=L} \left\{ dt = 0 \quad (1)
$$

where

 $K(t)$ is defined as:

$$
K(t) = \int_{t_r}^{t} k(t) dt
$$
 (II)

 $\varphi(x)$ is given by

$$
\varphi(x) = \begin{cases} \varphi_1(x), & 0 < x < \zeta(0) \\ \varphi_2(x), & \zeta(0) < x < L \end{cases} \tag{III}
$$

and $F(x, t)$ is any function which is continually differentiable, twice with respect to x and once with respect to τ , and such that

$$
F(0, \tau) = F(L, \tau) = F(x, \theta) = 0. \tag{IV}
$$

The results of [IS] and [20] concerning similar cases can be still utilized to show the existence and uniqueness of the generalized solution thus defined.

Thus the approximating problems are formulated as follows:

llows:
\n
$$
C^*(t) \frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left[k^*(t) \frac{\partial t}{\partial x} \right]
$$
\n(17)

with initial, and boundary conditions given by (2) , (3) , (5) and (6) . Each of these problems possesses unique classical solution $[16]$ which, according to points 1 and 2 and to the quoted results of [15, 20], as $\Delta t \rightarrow 0$ tends to the generalized solution of the Stefan problem.

The actual smoothing can be performed in many ways. Several shapes have been tested numerically and the choice does not seem to be critical.

A definition of $C^*(t)$ and $K^*(t)$ which works well and, owing to its simplicity, turns out to be very suitable for practical applications is described here.

Suppose that C_1 , C_2 , k_1 and k_2 do not depend on t, then in the interval: $t_f - \Delta t \leq t_f + \Delta t$ the following definitions may be assumed

$$
C^*(t) = \frac{\lambda}{2\Delta t} + \frac{C_1 + C_2}{2}
$$
 (18)

and

$$
k^*(t) = k_1 + \frac{k_2 - k_1}{2\Delta t} \left[t - (t_f - \Delta t) \right].
$$
 (19)

At this point it is worth mentioning that an important feature of the procedure outlined here is that the coefficient smoothing is carried out with respect to t and so it does not depend on whether the problems are one-dimensional or multi-dimensional. The extension to the multidimensional case therefore is straightforward and yields to equations which are formally analogous to equation (17). For example, in the three-dimensional case the equation corresponding to equation (17) is

$$
C^*(t)\frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left[k^*(t) \frac{\partial t}{\partial x} \right] + \frac{\partial}{\partial y} \left[k^*(t) \frac{\partial t}{\partial y} \right] + \frac{\partial}{\partial z} \left[k^*(t) \frac{\partial t}{\partial z} \right].
$$
 (20)

THE DIFFERENCE SCHEME

Only the numerical solution of equation (17) under boundary conditions of the first kind will be considered in detail here. However, since the three-time level implicit scheme employed here [4, 17] has been extended to the multi-dimensional case and to different boundary conditions [5], it can be said that, in principle, all the phasechange problems can be solved in this same way.

By using central difference operators the following approximation for equation (17) can be obtained

$$
C^*(T_i^h)(\mu\gamma)_\tau T_i^h = \frac{\Delta \tau}{\Delta x^2} \gamma_x [k^*(T_i^h)] \gamma_x \langle T_i^h \rangle \quad (21)
$$

where $\langle T_i^h \rangle$ is the average temperature:

$$
\langle T_i^h \rangle = \frac{1}{3} (T_i^{h+1} + T_i^h + T_i^{h-1}). \tag{22}
$$

Equation (21) can be rewritten as

$$
C^*(T_i^h) (T_i^{h+1} - T_i^{h-1})
$$

= $\frac{2}{3} \frac{\Delta \tau}{\Delta x^2} \{ k^+ [(T_{i+1}^{h+1} - T_i^{h+1})$
+ $(T_{i+1}^h - T_i^h) + (T_{i+1}^{h-1} - T_i^{h-1})]$
- $k^- [(T_i^{h+1} - T_{i-1}^{h+1}) + (T_i^h - T_{i-1}^h)]$
+ $(T_i^{h-1} - T_{i-1}^{h-1})]$ (23)

where

$$
k^{+} = k^{*}(T_{i+\frac{1}{2}}^{h}) \cong k^{*}\left(\frac{T_{i+1}^{h} + T_{i}^{h}}{2}\right)
$$

$$
k^{-} = k^{*}(T_{i-\frac{1}{2}}^{h}) \cong k^{*}\left(\frac{T_{i}^{h} + T_{i-1}^{h}}{2}\right).
$$
 (24)

The expressions (24) do not alter the order of accuracy of formula (23) and involve values of *T* at grid points only. Angther important feature of formula (23) is that the coefficients are computed at the intermediate time level: resorting to iterations is thus avoided, since the tridiagonal system of difference equations to be solved at each time step is linear.

When only data at $\tau = 0$ is given, in order to start the calculations it is necessary to obtain the data at $\tau = \Delta \tau$ from a two level formula of comparable accuracy.

It can be shown that the three-time level implicit scheme described here is unconditionally stable and convergent $[4, 17]$. By a Taylor's series expansion the local order of accuracy of equation (23) can be written as

$$
e_i^h = \frac{\Delta \tau^2}{6} \left(\frac{\partial^3 t}{\partial \tau^3} \right)_i^h - \frac{\Delta \tau^2}{3C^*} \frac{\partial}{\partial x} \left(k^* \frac{\partial^3 t}{\partial x \partial \tau^2} \right)_i^h
$$

$$
- \frac{\Delta x^2}{24C^*} \left[\frac{\partial}{\partial x} \left(k^* \frac{\partial^3 t}{\partial x^3} \right) + \frac{\partial^3}{\partial x^3} \left(k^* \frac{\partial t}{\partial x} \right) \right]_i^h + \dots = O(\Delta \tau^2 + \Delta x^2). \quad (25)
$$

RESULTS

The numerical method described in the previous sections has been checked against the results of available analytical solutions of onedimensional freezing problems [18]. A Fortran IV program, based on formula (23) has been written to calculate the temperature distribution in a slab with variable thermophysical properties.

The thermophysical properties used in the computations were those of the system water-ice. Constant values of the heat capacity and of the thermal conductivity were assumed in the solid and in the liquid region; in the phase-change zone the heat capacity and the thermal conductivity were smoothed according to definitions (18) and (19). Since freezing problems were treated, the phase front was taken to coincide with the isotherm $(t_f - \Delta t)$, corresponding to the lowest temperature end of the freezing zone.

Reference was made to a layer subjected to the following boundary conditions

$$
t_1(0, \tau) = t_a = \text{const}; \quad \tau > 0
$$
 (26)

$$
\frac{\partial t_2(L,\tau)}{\partial x} = 0; \qquad \tau > 0. \tag{27}
$$

First a simplified initial condition was considered assuming the temperature of the water to be at the freezing point, with no ice present:

$$
t_2(x, 0) = t_0 = t_f = \text{const};
$$

$$
\zeta(0) = 0 \le x \le L. \tag{28}
$$

FIG. 1. Interface histories.

In the calculations 41 equally spaced nodal points were used $(\Delta x = 0.0125 \text{ m}; L = 0.5 \text{ m})$ with time steps variable from 200 to 600 s but constant within each run. The phase change was usually assumed to take place in a temperature interval of 05 K, but the results obtained were rather insensitive to the particular choice operated. In Fig, 1 the computed phase front position curves are compared with the **corres**ponding analytical solution for different values of the initial "jump" $(t_0 - t_a)$ in the external surface temperature. In Fig. 2 the calculated temperature distributions at different time values are compared with the analytical solutions For

FIG. 2. Temperature distribution at different time values.

the particular case: $t_0 - t_a = 20$ K. The accuracy of the results plotted in Figs. 1 and 2 is always better than 1 per cent.

A phase change problem with the initial temperature of the water above the freezing point was then considered. The initial and boundary conditions were taken to coincide with the analytical solution at $\tau = 72000$ s yielded by the following boundary and initial conditions :

$$
t_1(0, \tau) = t_a = -20^{\circ}C; \qquad \tau > 0 \qquad (29)
$$

 $t_2(x, 0) = t_0 = 10^{\circ}\text{C}; \quad \xi(0) = 0 \le x \le L.$ (30)

In order to use in the comparison the analytical solution for a semi-infinite body, calculations were stopped at $\tau = 288000$ s as soon as the temperature $t(L, \tau)$ started to change appreciably.

When two phases are simultaneously present, as in this case, the choice of the temperature interval in which freezing is assumed to take place becomes critical. Numerical calculations have shown that good results are obtained only if the phase change interval embraces at least 2–3 nodes of the network along the x-axis $\lceil 22 \rceil$.

tion does not depend on the geometry considered, extension to multidimensional cases is straightforward.

As a final remark it is worth indicating that the assumption of pure conduction in the liquid phase is not always strictly correct, but experience has shown that for design calculations an equivalent thermal conductivity dependent on the Rayleigh number can be used when convection is of importance [14], avoiding thus changes in the problem formulation.

Moreover too large temperature intervals are not advisable since strong divergence from the original problem would arise. In the example considered here 81 equally spaced nodes were used $(\Delta x = 0.0125 \text{ m}; L = 1 \text{ m})$ and a phasechange interval of 2 K was assumed. The results obtained for the phase front histories and the temperature distributions are reported in Table 1 and in Table 2 respectively. The accuracy $(\approx 3$ per cent) is still well within the limits imposed for engineering calculations.

Run time for the Fortran program is about 20 s on a CDC 6600 computer with a grid of 41 nodal points and 1000 time steps.

CONCLUSIONS

The finite difference method presented in this paper has enabled to deal with melting and $\frac{7. \text{ J. R. CANNON and C. D. HILL, Existence, uniqueness}}{\text{stability and monotone dependence in a Stefan problem}}$ freezing problems. The results obtained have been shown to be sufficiently accurate for engineering use.

Reference has been made mostly to onedimensional cases but since the problem formula-

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SOLUTION NUMERIQUE DES PROBLEMES DE CHANGEMENT DE PHASE

Résumé—Un schéma implicite à trois niveaux de temps qui est inconditionnellement stable et convergent, est employé pour la solution numérique de problèmes de changement de phase sur la base d'une représentation analytique de l'effet de chaleur latente par une grande capacite caloritique sur un petit domaine de température. Puisque les coefficients dépendants de la température dans les équations paraboliques résultantes sont évalués au niveau intermédiaire de temps, on peut éviter la résolution compliquée d'un système d'équations algébriques non linéaires à chaque pas de temps. Les résultats numériques ainsi obtenus sont compares de maniere satisfaisante aux solutions analytiques connues.

NUMERISCHE LOSUNG VON PHASENANDERUNGSPROBLEMEN

Zusammenfassung—Ein Drei-Zeiten-Ebenen-System. das absolut stabil und konvergent ist, wird für die numerische Lösung von Phasenänderungsproblemen verwendet.

Für kleine Temperaturbereiche wird die latente Wärme durch eine grosse Wärmekapazität angenähert. Die temperaturabhängigen Koeffizienten in den resultierenden parabolischen Gleichungen wurden auf einer Zwischenzeitebene abgeschätzt, womit die Schwierigkeit, eine Reihe von nichtlinearen algebraischen Gleichungen bei jedem Zeitschritt zu lösen, vermieden ist. Die so erhaltenen numerischen Lösungen zeigten mit den verfügbaren analytischen Lösungen zufriedenstellende Übereinstimmung.

ЧИСЛЕННОЕ РЕШЕНИЕ ЗАДАЧ О ФАЗОВЫХ ПЕРЕХОДАХ

Аннотация—Для численного решения задач о фазовых переходах используется абсолютно устойчивая и сходящаяся неявная схема с тремя временными уровнями (трехслойная схема). Метод состоит в том, что скрытый тепловой эффект аппроксимируется большим значением теплоемкости в малом температурном диапазоне. Поскольку зависящие от температуры коэффициенты в параболических уравнениях рассчитываются на промежуточном временном уровне, можно избежать трудности peшения системы нелинейных алгебраических уравнений на каждом временном уровне. Полученные таким способом численные результаты удовлегворительно согласуются с имеющимися аналитическими решениями.