Int J Fract (2008) 150:227–240
DOI 10.1007/s10704-008-9223-5

ORIGINAL PAPER

Dynamic fracture as a process of nonlinear damage wave propagation

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Received: 9 January 2008 / Accepted: 17 May 2008 / Published online: 29 July 2008
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Abstract A new approach describing the dynamic fracture as a process of nucleation and subsequent propagation of a nonlinear wave of microfracture is proposed. The equation describing the microfracture evolution is derived from the transfer equation and a stochastic diffusion-type description of damage redistribution. The physical meaning of the corresponding parameters is clarified by the mass conservation and the incubation time criterion of fracture. Finally the process of dynamic macrocrack nucleation is simulated.

Keywords Dynamic fracture · Fracture wave · Damage evolution · Dynamic crack propagation · Fracture simulation

1 Introduction

Classical quasistatic fracture criteria are usually represented in the terms of instant values of the local stresses (or the stress intensity factor for the crack problems) at the supposed fracture point. In contrast, the dynamic fracture modeling is principally based on a characteristic time of microfracture and corresponding micro-relaxation (micro-redistribution) processes preceding the macro-fracture event. In order to account the integral contribution of such processes into the dynamic fracture phenomenon an incubation time approach was proposed in Petrov and Utkin (1989); Morozov et al. (1990) and developed as a "quantized" fracture mechanics by Petrov (1991, 1996, 2004). Introducing a characteristic time of micro-relaxation processes (the incubation time) as a structural material parameter together with the static fracture toughness it is possible to state the incubation time based criterion of macroscopic fracture (e.g. see Petrov et al. 2003; Petrov and Sitnikova 2004; Pugno 2006; Bratov and Petrov 2007a, b) that turned out to be very powerful to describe experimentally observed effects

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of dynamic crack growth initiation and propagation (Homma et al. 1983; Ravi-Chandar and Knauss 1984a, b). But a continual description of fracture evolution and corresponding incubation process at the microscopic scale level has not been provided.

To describe the microfracture evolution (including the processes of nucleation, interaction and following coalescence of microfracture—microcracks, microdamage, vacancies and so on) we will define the function describing an instant local microfracture state (the damage function). Then we will clarify the behaviour of damage function based on the transfer equation, the principles of damage mechanics and the incubation time approach. The detailed analysis will be conducted for the one-dimensional problem. Finally the process of dynamic crack nucleation will be simulated starting from the experimental results.

2 Diffusion description of dynamic fracture

Firstly let us derive the kinetic equation describing the microfracture process in the form of transfer equation. We fix an arbitrary stationary domain Ω inside the considered solid and introduce the damage function $\theta(\bar{r}, t) \in [0, 1]$ to characterize the relative volume of microfracture (microdamage) in solid's mass unit in the neighborhood of every point $\bar{r} \in \Omega$. Then $\theta = 0$ corresponds to the intact material whereas $\theta = 1$ to the local state of macroscopic fracture. And $\theta_\Omega(t) = \int_\Omega \rho(\bar{r})\ \theta(\bar{r}, t)\ d\bar{r}$ describes the evolution of local material density in Ω during the microfracture processes, where ρ is the local density of the initial intact material. We can apply the transfer principle for θ_Ω: the change of θ_Ω inside of Ω is caused by a flux of microfracture J_{θ_Ω} through the boundary $\partial\Omega$ and by an internal sources of microfracture Σ_{θ_Ω}. That is

$$\frac{d}{dt}\theta_\Omega(t) = -J_{\theta_\Omega} + \Sigma_{\theta_\Omega}. \tag{2.1}$$

Let $\bar{j}_\theta d\bar{s}$ denotes the elementary flux of θ through the area $d\bar{s}$ having the outer normal $\bar{n}$; similarly $\sigma_\theta d\bar{r}$ defines the rate of an internal sources of θ in the neighborhood of point $d\bar{r}$ inside Ω. Then, by the divergence theorem, we obtain

$$J_{\theta_\Omega} = \int\limits_{\partial\Omega} \bar{j}_\theta d\bar{s} = \int\limits_{\Omega} \nabla \cdot \bar{j}_\theta d\bar{r} \tag{2.2}$$

and

$$\Sigma_{\theta_\Omega} = \int\limits_{\Omega} \sigma_\theta d\bar{r}. \tag{2.3}$$

Owing to the fact that the domain Ω is fixed in space we have

$$\frac{d}{dt}\theta_\Omega = \frac{d}{dt}\int\limits_{\Omega} \rho\theta d\bar{r} = \int\limits_{\Omega} \frac{\partial}{\partial t}(\rho\theta)\, d\bar{r}, \tag{2.4}$$

and due to arbitrary choice of Ω, Eq. 2.1 can be rewritten as

$$\frac{\partial}{\partial t}(\rho\theta) + \nabla \cdot \bar{j}_\theta = \sigma_\theta. \tag{2.5}$$

Supposing the flux of microfracture over the boundary $\partial\Omega$ to be totally determined by a diffusion-type processes of microfracture redistribution we can use the Fick's law

$\bar{j}_\theta = -D(t) \nabla(\rho\theta)$. The function $D(t)$ might be termed the relaxation factor. It has the physical meaning of the rate of relaxation processes at the microscale.

Further we will not go beyond the one-dimensional case. Then, neglecting the variation of density of an undamaged part of solid, Eq. 2.5 is reduced to

$$\frac{\partial\theta}{\partial t} = D(t) \frac{\partial^2\theta}{\partial x^2} + f(\theta, x, t), \quad \text{where } f(\theta, x, t) = \sigma_\theta/\rho. \tag{2.6}$$

Equation 2.6 describes the microfracture evolution in the form of diffusion equation. This equation involves two functions, namely the relaxation factor D and the microfracture source function f, whose expressions with reference to the fracture process have to be clarified. Following this aim, we examine the one-dimensional process of microfracture accumulation from the viewpoint of damage mechanics.

In the general form of damage equation

$$\frac{\partial\theta}{\partial t} = g(\theta, x, t) + f(\theta, x, t) \tag{2.7}$$

the functional $f(\theta, x, t)$ describes the macroscopically uniform process of microfracture accumulation whereas $g(\theta, x, t)$ describes a local stochastic (fluctuating) processes around a point x, namely the local processes of relaxation (redistribution) of microfracture. Let $P(x, t)\,dx$ to be the probability of defect "migration" from the point x within a distance dx at the time t. Then we can write

$$g(\theta, x, t) = \psi \left(\int_{-\infty}^{+\infty} \theta(\zeta, t) P(\zeta - x, t) d\zeta - \theta(x, t) \right), \tag{2.8}$$

where ψ is a constant characterizing the intensity of microfracture redistribution. Since $\int_{-\infty}^{+\infty} P(\zeta, t) d\zeta = 1$ then $\int_{-\infty}^{+\infty} \zeta P(\zeta, t) d\zeta = 0$ as the integral of an odd function. Denoting $R(t) = \sqrt{\int_{-\infty}^{+\infty} \zeta^2 P(\zeta, t) d\zeta}$ and expanding the function θ into a Taylor series up to the second order terms

$$\theta(\zeta, t) = \theta(x, t) + \frac{\partial\theta(x, t)}{\partial x}(\zeta - x) + \frac{1}{2}\frac{\partial^2\theta(x, t)}{\partial x^2}(\zeta - x)^2 + o(\zeta - x)^2 \tag{2.9}$$

we can rewrite Eq. 2.8 as $g(\theta, x, t) = \frac{\psi}{2} R^2(t) \frac{\partial^2\theta(x,t)}{\partial x^2}$. Then, Eq. 2.7 can be reduced to

$$\frac{\partial\theta}{\partial t} = \frac{\psi R^2(t)}{2} \frac{\partial^2\theta}{\partial x^2} + f(\theta, x, t). \tag{2.10}$$

This equation has the same form of Eq. 2.6. Comparing them we can express the relaxation factor as

$$D(t) = \frac{\psi R^2(t)}{2} \tag{2.11}$$

and conclude that the source function $f(\theta, x, t)$ in Eq. 2.6 is the term describing the uniform process of microfracture accumulation at the macroscale. We will obtain its exact expression based on the principle of mass conservation.

3 Uniform process of microfracture accumulation

Let us choose a sufficiently small portion inside the considered solid to be sure that its density is changing homogeneously during the damage accumulation process. Its mass is denoted as m, its volume before deformation is V_0 whereas the total volume of microfracture (microdefects) accumulated inside the chosen portion is V_*. Thus, during the damage process its volume changes as $V = V_0 + V_*$. The change of volume is obviously accompanied by a variation of local density ρ, described by the mass conservation

$$\frac{1}{\rho}\frac{d\rho}{dt} = -div\bar{v}, \tag{3.1}$$

where $\bar{v}$ is a local velocity of material particles.

From the other side we can express the local density as $\rho = \frac{dm}{dV} = \frac{dm}{dV_0}\frac{dV_0}{dV} = \frac{dm}{dV_0}\left(1 - \frac{dV_*}{dV}\right)$. Introducing the damage parameter $\theta = \frac{dV_*}{dV}$ and setting $\rho_0 = \frac{dm}{dV_0}$ we obtain

$$\rho = \rho_0 (1 - \theta). \tag{3.2}$$

Substituting expression (3.2) into Eq. 3.1 yields

$$\frac{d\theta}{dt} = (1 - \theta)\ div\bar{v}. \tag{3.3}$$

Equation 3.3 represents the mass conservation law in the form of kinetic damage equation. To approximate the divergence of local velocity belonging to the right side of Eq. 3.3 let us expand it into a power series of θ

$$div\ \bar{v} = C_0 + C\theta + \bar{o}(\theta) + \cdots. \tag{3.4}$$

Omitting the higher terms in expansion (3.4) and noting the absence of volume expansion for the intact material ($div\ \bar{v}|_{\theta=0} = 0$), Eq. 3.3 becomes

$$\frac{d\theta}{dt} = C\theta (1 - \theta). \tag{3.5}$$

Here $C = C(x, t)$ is an unknown function. In the particular case of $C = const$, Eq. 3.5 represents the well-known simplest logistic equation, which is often used in damage mechanics to describe the process of damage accumulation.

Recollecting the arguments mentioned above it is suggested

$$f(\theta, x, t) = C(x, t)\,\theta (1 - \theta). \tag{3.6}$$

It remains to define the exact form of microfracture source intensity $C(x, t)$. When $C(x, t) = 0$, just a microfracture redistribution takes place and a new microfracture is not provided. Besides that, it is natural to suppose that the fracture is intensified under the strain and, hence, the intensity of microfracture source has to be determined by the rate of stress field change (or by the rate of stress intensity factor change in the case of macrocrack existence). Taking into account the incubation time phenomenon, according to Kashtanov and Petov (2007), we can define the intensity of microfracture source as

$$C(x, t) = \frac{1}{F_c\tau}(F(t) - F(t - \tau)). \tag{3.7}$$

Here $F(t)$ is the local intensity of stress field and F_c represents its critical value. In the crack problems $F(t)$ coincides with the stress intensity factor $F(t) = K_1(t)$ and F_c is the static

fracture toughness. The structural material parameter τ in Eq. 3.7 is the structural (incubation) time, which has the meaning of a characteristic time of micro-relaxation processes and could be measured experimentally (e.g. see Morozov and Petrov 2000).

4 Model validation

Let us consider a particular case of Eq. 2.6 assuming $D = const$ and introducing the new dimensionless variables $X = x/\sqrt{\tau D}$ and $T = t/\tau$. Then, Eq. 2.6 takes the dimensionless form

$$\frac{\partial \theta}{\partial T} = \frac{\partial^2 \theta}{\partial X^2} + \Phi(\theta, X, T), \quad \Phi(\theta, X, T) = \frac{F(T) - F(T-1)}{F_c}\theta(1-\theta). \tag{4.1}$$

In general this equation can not be solved analytically. Nevertheless, in the particular case when $F(T)$ increases at constant velocity, Eq. 4.1 becomes the classical Kolmogorov-Petrovsky-Piskunov equation, see Kolmogorov et al. (1937)

$$\frac{\partial \theta}{\partial T} = \frac{\partial^2 \theta}{\partial X^2} + \Phi(\theta), \quad \Phi(\theta) = \alpha\,\theta(1-\theta),$$
$$\text{where } \alpha = \frac{F(T) - F(T-1)}{F_c} = const > 0. \tag{4.2}$$

It is known that this equation admits the solutions in the form of a kink-type autowave. Indeed, Eq. 4.2 is invariant with respect to translation by X and T. Therefore, imposing the appropriate boundary conditions, we can obtain the solutions of this equation which are not depending on the initial condition. It means that after some time period the solution "forgets" the initial condition and goes into the steady-state when the wave front remains the same with time and the front profiles remain self-similar (see also Carpinteri 1994). Supposing that the wave front moves with a constant velocity λ from right to left and interesting in the autowave solution $\theta = \theta(X - \lambda T)$, we can reduce Eq. 4.2 to the ordinary differential equation:

$$\varphi\left(\lambda + \frac{d\varphi}{d\theta}\right) = -\alpha\,\theta(1-\theta), \quad \text{where } \varphi(\theta) = \frac{d\theta}{d(X - \lambda T)}. \tag{4.3}$$

The problem (4.3) is known from the theory of laminar flame spreading (e.g. see Zeldovich et al. 1985). In particularly, it was proved that under the boundary conditions $\varphi(0) = 0$ and $\varphi(1) = 0$, it has an infinite set of solutions with the corresponding spectrum of wave velocities $\lambda \geq 2\sqrt{\alpha}$. Moreover $\theta = 0$ and $\theta = 1$ are the lower and upper asymptotes of its solutions. Accordingly, we have verified that, at least in the case when $F(T)$ increases at the constant velocity, the obtained equation can be used to describe the propagation of fracture surface as a nonlinear microfracture wave.

It is easy to see that $\theta = 0$ and $\theta = 1$ also bound the solutions of Eq. 4.1. Indeed, when $\theta(X_0, T_0) = 0$ or $\theta(X_0, T_0) = 1$ then $\Phi(\theta, X_0, T_0) = 0$ and Eq. 4.1 becomes purely diffusive $\theta_T(X_0, T_0) = \theta_{XX}(X_0, T_0)$.

For further investigation of Eq. 4.1 the finite-difference scheme of forth order of approximation is designed (see Appendix 1). Having the numerical solution of Eq. 4.1, we can define the dimensionless front velocity $V(T)$ of the microfracture wave. Coming back to the dimension variables we obtain

$$v(t) = \frac{dx}{dt} = V(T)\sqrt{\frac{D}{\tau}}, \tag{4.4}$$

where $v(t)$ is the experimentally measured velocity of macrocrack. Accordingly, the value of relaxation factor is

$$D = \tau \left(\frac{v(t)}{V(T)} \right)^2 . \tag{4.5}$$

Expression (4.5) completes the model for the particular case of the constant rate of microfracture relaxation during fracture process.

Let us note that expression (4.4) gives an important qualitative result: the dynamic crack speed decreases by increasing the square root of incubation time as $v \sim \tau^{-1/2}$. This result could be useful to design the materials which are able to effectively resist against the dynamic fracture.

5 Numerical example

We will simulate the process of dynamic crack nucleation rather than its propagation because in this case the microfracture source function $\Phi(\theta, X, T)$ could have a very simple form. The problem of macrocrack propagation can be investigated by the same procedure but with another and more complicated source function.

Let us consider an elastic plane with an initial semi-infinite rectilinear crack $x \in (-\infty, 0]$. The crack faces are subjected to a symmetric shock loading $p(t) = PtH(t)$, where $P = const$ is the loading rate and $H(\varsigma) = \begin{cases} 0, & \varsigma < 0 \\ 1, & \varsigma \geq 0 \end{cases}$ is the unit step function. In this problem the stress intensity factor is defined as $K_1(t) = 2/3 P \varphi(c_1, c_2)\ t^{3/2} H(t)$ (Petrov and Sitnikova 2004), where c_1 and c_2 are the velocities of the longitudinal and transverse waves in the solid and $\varphi(c_1, c_2) = 4\frac{c_2}{c_1}\sqrt{\frac{c_1^2 - c_2^2}{\pi\, c_1}}$. Then, in compliance with Eq. 4.1 we can write the microfracture source function as

$$\Phi(\theta, X, T) = \frac{2}{3}\frac{P}{K_{1c}} \varphi(c_1, c_2)\ \tau^{3/2} \theta(1-\theta) \left(T^{3/2} H(T) - (T-1)^{3/2} H(T-1) \right). \tag{5.1}$$

Accordingly the analysis conducted in Kashtanov and Petov (2007), we can define the time to crack start t_* (the time passed from the moment of loading application till the moment of macrocrack start) from

$$P = \frac{15\tau K_{1c}}{4\varphi} \left(t_*^{5/2} - (t_* - \tau)^{5/2} \right)^{-1} . \tag{5.2}$$

Therefore

$$\Phi(\theta, X, T) = \frac{5}{2} \frac{T^{3/2} H(T) - (T-1)^{3/2} H(T-1)}{T_*^{5/2} - (T_* - 1)^{5/2}} \theta(1-\theta), \tag{5.3}$$

where $T_* = t_*/\tau$ is the dimensionless time to crack start.

The right side of expression (5.3) does not depend on x. Much more important that $\Phi(\theta, X, T)$, as well as the corresponding solution of Eq. 4.1, is fully determined by only one parameter—the time to crack start. That is, for every value of T_* we have the same dimensionless solutions $\theta(X, T)$, regardless of the material properties. It makes the problem of crack nucleation much simpler than the problem of its subsequent propagation. The difference in

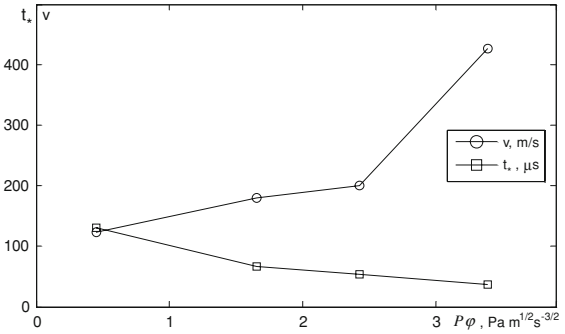

Fig. 1 The experimental values of the initial crack velocity v and the corresponding time to crack start t_* for different "reduced" loading rates $P\varphi$

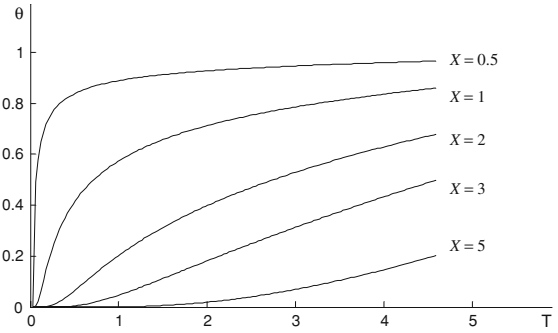

Fig. 2 The dependence of the damage function θ on time during the crack nucleation process in different points at the given distances from the initial crack

the material properties is accounted by the inverse transformation to dimensional variables through the values of τ and D.

We simulate the process of dynamic crack nucleation at the extension of initial crack, namely inside the interval $[0, X_N]$ sufficiently wide to neglect the effect of a right boundary condition. The initial and boundary conditions are stated in the form

$$\theta(X, 0) = 1 - H(X), \quad \theta(0, T) = 1, \quad \theta(X_N, T) = 0. \tag{5.4}$$

Let us consider the experimental data from Ravi-Chandar and Knauss (1984a, b) obtained on Homalite-100 ($K_{1c} = 0.48\,\mathrm{MPa\,m^{1/2}}$ and $\tau = 8\,\mu\mathrm{s}$). In Fig. 1 the experimental results related to the time to crack start t_* (squares) as well as the initial velocity of macrocrack v (circles) are plotted versus four different "reduced" loading rates $P\varphi$.

Figure 2 displays the microfracture accumulation during the crack nucleation process for the experimental value of $T_* = 4.616$ ($t_* = 37\,\mu\mathrm{s}$) in different points close to the tip of initial crack. Apparently, the dynamic macrocrack is nucleated up to the time T_*.

The dynamic evolution of damage wave front for the same experimental value of $T_* = 4.616$ ($t_* = 37\,\mu\mathrm{s}$) is presented in Fig. 3. The initial crack is continuously diffusing and the fracture process zone (pre-crack zone) corresponding to $0 < \theta < 1$ is formed.

Figure 4 shows the computed dimensionless velocities V of the microfracture wave front (circles) and the values of relaxation factor D (squares), defined in compliance with the relation (4.5), for different experimental values of the time to crack start.

As shown in the Fig. 4 the assumption of constant relaxation factor is defensible in the considered problem. But let make a reference how to take into account the dependence of relaxation factor on the stress state (and, hence, on time), for example, to simulate the dynamic fracture under a pulsating load. Supposing $D = D(t)$ and transferring to the dimensionless

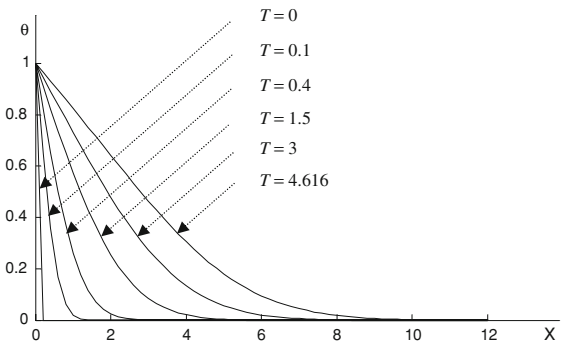

Fig. 3 The dependence of the damage function θ on the distances from the initial crack tip in the given time moments

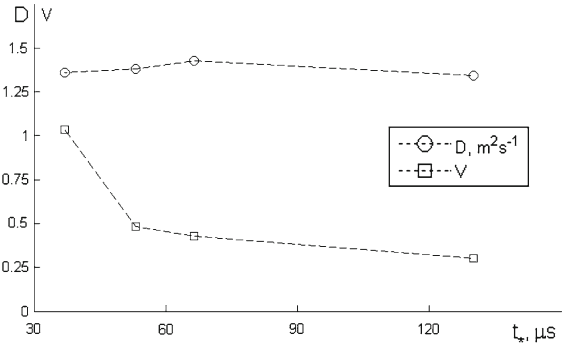

Fig. 4 The dependences of relaxation factor D and dimensionless crack velocity V on the time to crack start t_*

variables in Eq. 2.6 we will not succeed in excluding the dependence $D(t)$ from the final equation. Thus, we are obliged to construct a finite-difference scheme with the varied time step and to determine the dependence of relaxation factor on time before starting the simulation. For example, we can determine this dependence having an experimental data describing the morphology of fractured surface or the size of fracture process zone. Indeed, the relaxation factor determines the characteristic redistribution area of microfracture whereas the incubation time is the characteristic time of microfracture redistribution processes. Then, the magnitude $\sqrt{D(t)\,\tau}$ determines the characteristic linear size of the fracture process zone accompanying the crack propagation.

6 Conclusion

The equation of dynamic fracture evolution as a process of nucleation and subsequent coalesce of microfracture has been derived. Relations between the model parameters and the macroscopic physical characteristics of fracture process (the static fracture toughness and the incubation time) have been defined from the principles of damage mechanics and incubation time approach. Obtained equation describes the propagation of macrocrack as a nonlinear microfracture wave. It was shown that in the case of uniformly increasing stress field (or stress intensity factor) the model can be reduced to the well-known Kolmogorov-Petrovsky-Piskunov equation.

The numerical finite-difference scheme of the forth order of approximation was developed. The stability and convergence of this scheme was proved. For the one-dimensional case,

corresponding to the propagation of macrocrack under the assumption of "independent" microfracture relaxation, the equation has been numerically solved. A process of dynamic macrocrack nucleation was simulated using experimental data related to the time to crack start and the initial crack velocity. The model also describes the crack propagation following the nucleation stage.

Acknowledgements The authors acknowledge the support of the Russian Federal Agency of Science and Innovations (State Contract 02.444.11.7239) and of the President of Russian Federation (Grant MK-3151.2005.1).

Appendix 1: The finite-difference scheme

The equation to be solved is

$$\frac{\partial\theta\,(X,T)}{\partial T}=\frac{\partial^2\theta\,(X,T)}{\partial X^2}+\Phi(\theta,X,T) \tag{7.1}$$

with the initial and boundary conditions given by

$$\theta\,(X,0)=\Psi\,(X)\,,\quad A_0\frac{\partial\theta\,(0,T)}{\partial X}+B_0\,\theta(0,T)=C_0\,(T)\,,$$
$$A_N\frac{\partial\theta\,(X_N,T)}{\partial X}+B_N\theta\,(X_N,T)=C_N\,(T). \tag{7.2}$$

The approximate solution $\theta\in[0,\ \infty)$ is built inside the domain $(X,T)\in[0,X_N]\times[0,T_M]$, in the vertexes of rectangles of the dimension $h\times s$, which compose the grid of size $0\ldots N\times 0\ldots M$.

Let us rewrite Eq. 7.1 in the following concise form

$$\Lambda\theta=\Phi\,(\theta,X,T),\quad \text{where } \Lambda\theta=\theta_T-\theta_{XX}, \tag{7.3}$$

and fix the relation between the grid dimensions according to

$$k=s/h^2=const. \tag{7.4}$$

We would like to construct the six-nodes implicit finite-difference scheme to approximate the solution of Eq. 7.3 with the accuracy $O\left(s^2+h^4\right)=O\left(h^4\right)$. That is, in every grid point we have to find the approximation polynomial

$$\Lambda_h\theta^{i,j}=a_1\theta^{i-1,j}+a_2\theta^{i,j}+a_3\theta^{i+1,j}+a_4\theta^{i-1,j+1}+a_5\theta^{i,j+1}+a_6\theta^{i+1,j+1}, \tag{7.5}$$

where $a_1,\ \ldots,\ a_6$ are the constant coefficients identical through all the grid and $\theta^{i,j}=\theta\,(ih,js)$ is the value of the required solution in the corresponding grid point (see Fig. 5).

Thus the finite-difference equation corresponding to Eq. 7.3 can be written as

$$\Lambda_h\theta^{i,j}=\Phi\left(\theta^{i,j},ih,js\right)+O\left(h^4\right),\quad i=0,1,\ldots,N,\quad j=0,1,\ldots,M. \tag{7.6}$$

To construct an approximated solution $\theta^{i,j}$ we have to match the coefficients $a_1,\ \ldots,\ a_6$ to provide the desirable accuracy. For simplicity, let us impose the following conditions: $a_1=a_3$ and $a_4=a_6$. Then, using the expansion into a Taylor series we can obtain the expression for $\Lambda_h\theta^{i,j}$ in any fixed grid point $(i,\ j)$:

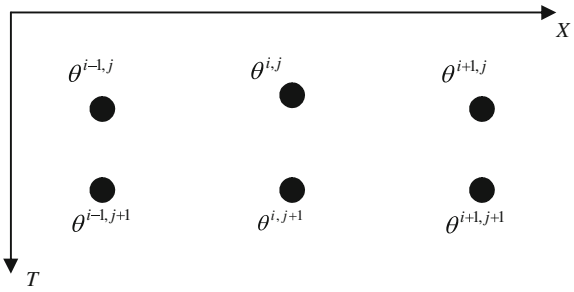

Fig. 5 The parabolic equation stencil

$$\begin{aligned}\Lambda_h\theta^{i,j} &= (2a_1 + a_2 + 2a_4 + a_5)\,\theta^{i,j} + h^2\,(a_1 + a_4)\,\theta^{i,j}_{XX} + \frac{h^4}{12}\,(a_1 + a_4)\,\theta^{i,j}_{XXXX} \\ &+ kh^2\,(2a_4 + a_5)\,\theta^{i,j}_T + \frac{k^2h^4}{2}\,(2a_4 + a_5)\,\theta^{i,j}_{TT} + kh^4a_4\theta^{i,j}_{XXT} \\ &+ O\left(a_1h^6, a_4h^6, (a_4 + a_5)\,k^3h^6, a_4k^2h^6, a_4kh^6\right) \end{aligned} \tag{7.7}$$

Due to $\theta_T = \Lambda\theta + \theta_{XX}$ we have

$$\theta_{XXT} = \theta_{TXX} = \Lambda\theta_{XX} + \theta_{XXXX} \text{ and } \theta_{TT} = (\Lambda\theta + \theta_{XX})_T = \Lambda\theta_T + \Lambda\theta_{XX} + \theta_{XXXX}$$

and Eq. 7.7 becomes

$$\begin{aligned}\Lambda_h\theta^{i,j} &= (2a_1 + a_2 + 2a_4 + a_5)\,\theta^{i,j} + h^2\,(a_1 + a_4 + k\,(2a_4 + a_5))\,\theta^{i,j}_{XX} \\ &+ \frac{h^4}{2}\left(\frac{a_1 + a_4}{6} + 2ka_4 + k^2\,(2a_4 + a_5)\right)\theta^{i,j}_{XXXX} \\ &+ kh^2\,(2a_4 + a_5)\,\Lambda\theta^{i,j} + \frac{k^2h^4}{2}\,(2a_4 + a_5)\,\Lambda\theta^{i,j}_T \\ &+ kh^4\left(a_4 + \frac{k}{2}\,(2a_4 + a_5) +\right)\Lambda\theta^{i,j}_{XX} \\ &+ O\left(a_1h^6, a_4h^6, (a_4 + a_5)\,k^3h^6, a_4k^2h^6, a_4kh^6\right) \end{aligned} \tag{7.8}$$

Therefore, to obtain the required accuracy we have to demand (e.g. see Godunov and Ryaben'kii 1987)

$$\begin{cases} 2a_1 + a_2 + 2a_4 + a_5 = 0 \\ a_1 + a_4 + k\,(2a_4 + a_5) = 0 \\ \frac{a_1 + a_4}{6} + 2ka_4 + k^2\,(2a_4 + a_5) = 0 \end{cases}. \tag{7.9a}$$

Using the option to specify the closure condition to combined Eqs. 7.9a we impose

$$kh^2\,(2a_4 + a_5) = 1. \tag{7.9b}$$

By solving the system of algebraic Eqs. 7.9 we obtain

$$\begin{aligned} a_1 = a_3 &= -\frac{1}{2h^2}\left(1 + \frac{1}{6k}\right), \quad a_2 = \frac{1}{h^2}\left(1 + \frac{1}{6k} - \frac{1}{k}\right), \\ a_4 = a_6 &= -\frac{1}{2h^2}\left(1 - \frac{1}{6k}\right), \quad a_5 = \frac{1}{h^2}\left(1 - \frac{1}{6k} + \frac{1}{k}\right). \end{aligned} \tag{7.10}$$

Substituting expressions (7.10) into Eq. 7.8 and using the notation (7.3) yields

$$\Lambda_h \theta^{i,j} = \Phi^{i,j} + \frac{kh^2}{2}\left(\Phi_T^{i,j} + \frac{1}{6k}\Phi_{XX}^{i,j}\right) + O\left(h^4\right), \quad \Phi^{i,j} = \Phi\left(\theta^{i,j}, ih, js\right). \tag{7.11}$$

Expanding the derivatives of $\Phi^{i,j}$ into a Taylor series we finally obtain

$$\Lambda_h \theta^{i,j} = \Phi_0^{i,j} + O\left(h^4\right), \quad \text{where } \Phi_0^{i,j} = \frac{4}{3}\Phi^{i,j} + \frac{1}{12}\left(\Phi^{i+1,j} + \Phi^{i-1,j} - 6\Phi^{i,j-1}\right). \tag{7.12}$$

Thus, Eq. 7.1 becomes

$$a_4\theta^{i-1,j+1} + a_5\theta^{i,j+1} + a_6\theta^{i+1,j+1} = -a_1\theta^{i-1,j} - a_2\theta^{i,j} - a_3\theta^{i+1,j} + \Phi_0^{i,j}. \tag{7.13}$$

It is easy to see that the constructed scheme is a refined modification of the Crank-Nicholson scheme (e.g. see Godunov and Ryaben'kii 1987):

$$\frac{\theta^{i,j+1} - \theta^{i,j}}{s} = \mu\frac{\theta^{i-1,j+1} - 2\theta^{i,j+1} + \theta^{i+1,j+1}}{h^2} + (1-\mu)\frac{\theta^{i-1,j} - 2\theta^{i,j} + \theta^{i+1,j}}{h^2}, \quad \text{where } \mu = \frac{1}{2}\left(1 - \frac{1}{6k}\right).$$

Finalizing the implicit difference formula the initial and boundary conditions (7.2) can be rewritten, using the expansion into a Taylor series, as

$$\begin{aligned}
&\theta^{i,0} = \Psi(ih), \\
&-\frac{A_0}{2h}\theta^{2,j} + \frac{4A_0}{2h}\theta^{1,j} + \left(B_0 - \frac{3A_0}{2h}\right)\theta^{0,j} = C_0(js), \\
&\frac{A_N}{2h}\theta^{N-2,j} - \frac{4A_N}{2h}\theta^{N-1,j} + \left(B_N + \frac{3A_N}{2h}\right)\theta^{N,j} = C_N(js).
\end{aligned} \tag{7.14}$$

Finally, Eqs. 7.13 and 7.14 (for every value of $j > 1$) can be put in the following matrix form

$$\mathrm{A}\Theta^{j+1} = -\mathrm{B}\Theta^{j} + Y^{j}, \tag{7.15}$$

where

$$\mathrm{A} = \begin{pmatrix}
B_0 - \frac{3A_0}{2h} & \frac{4A_0}{2h} & -\frac{A_0}{2h} & 0 & \dots & 0 \\
a_4 & a_5 & a_6 & 0 & \dots & 0 \\
0 & a_4 & a_5 & a_6 & \dots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \dots & 0 & a_4 & a_5 & a_6 \\
0 & \dots & 0 & \frac{A_N}{2h} & -\frac{4A_N}{2h} & B_N - \frac{3A_N}{2h}
\end{pmatrix}_{(N+1)\times(N+1)}, \tag{7.16a}$$

$$\mathrm{B} = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ a_1 & a_2 & a_3 & 0 & \dots & 0 \\ 0 & a_1 & a_2 & a_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & a_1 & a_2 & a_3 \\ 0 & \dots & 0 & 0 & 0 & 0 \end{pmatrix}_{(N+1)\times(N+1)}, \quad \Theta^j = \begin{pmatrix} \theta^{0,j} \\ \theta^{1,j} \\ \theta^{2,j} \\ \vdots \\ \theta^{N-1,j} \\ \theta^{N,j} \end{pmatrix}_{N+1},$$

$$Y^j = \begin{pmatrix} C_0\,(js) \\ \Phi_0^{1,j} \\ \Phi_0^{2,j} \\ \vdots \\ \Phi_0^{N-1,j} \\ C_N\,(js) \end{pmatrix}_{N+1}. \tag{7.16b}$$

The solution for $j = 0$ is given by the initial condition (7.14) but for $j = 1$ it has to be defined from a different considerations. The reason of picking out the case of $j = 1$ is obvious. The relation (7.12) shows that the value $\Phi_0^{i,0}$ depends on $\Phi^{i,-1}$, which is undetermined. Nevertheless we can define the value of $\theta^{i,1}$ directly from the initial condition (7.14), which can be written as $\theta_{XX}^{i,0} = \Psi_{XX}^{i}$. Using a Taylor expansion we have $\theta^{i,1} = \theta^{i,0} + s\theta_T^{i,0} + O\left(s^2\right)$, and it follows from Eq. 7.3 that $\theta_T^{i,0} = \Lambda\theta^{i,0} + \theta_{XX}^{i,0}$ and $\Lambda\theta^{i,0} = \Phi^{i,0}$. Therefore, the approximate solution for $j = 1$ can be expressed as

$$\theta^{i,1} = \Psi^i + kh^2\left(\Phi^{i,0} + \Psi_{XX}^{i}\right) + O\left(h^4\right), \quad i = 0, 1, \dots, N \tag{7.17}$$

Thus we have constructed the implicit numerical scheme of forth order of approximation to solve the nonlinear parabolic Eqs. 7.1–7.2. Further considerations are concerned to a particular case of our interest corresponding to the fracture process, characterized by $\theta\,(x, t) \in [0, 1]$.

Now let us prove the stability of constructed approximation scheme and the convergence of numerical solution to the exact one. We are going to carry out the proof for the case $1/6 \le k \le 5/6$. It is sufficiently general for applications and in this case the proof is extremely simple. Firstly let rewrite the problem described by Eqs. 7.1 and 7.2 in the following form

$$\begin{aligned} \Lambda_h\theta^{i,j} &= \Phi_0^{i,j} \\ \theta^{i,0} &= \Psi^i \end{aligned} \tag{7.18}$$

where $\Lambda_h\theta^{i,j}$ are defined by relations (7.5) and (7.10), $\Phi_0^{i,j}$ is determined by Eq. 7.12 and $\Psi^i = \Psi\,(ih)$. It is easy to show that if the inequality

$$\max_j \sup_i \left|\theta^{i,j}\right| \le C\left(\sup_{i,j}\left|\Phi_0^{i,j}\right| + \sup_i\left|\Psi^i\right|\right) \tag{7.19}$$

is valid then the numerical scheme is stable (e.g. see Godunov and Ryaben'kii 1987). Here C is some positive constant. For the considered case $1/6 \le k \le 5/6$ the coefficients are limited by

$$\begin{aligned} a_1, a_3 &\in \left[-\frac{1}{h^2}, -\frac{3}{5h^2}\right], \quad a_2 \in \left[-\frac{4}{h^2}, 0\right], \quad a_4, a_6 \in \left[-\frac{2}{5h^2}, 0\right], \\ a_5 &\in \left[\frac{2}{h^2}, \frac{6}{h^2}\right]. \end{aligned} \tag{7.20}$$

The codomain of the approximated solution is the interval [0, 1], and using Eq. 7.5 we obtain the estimation $\left|\Lambda_h \theta^{i,j}\right| \geq \left|a_2 \theta^{i,j} + a_5 \theta^{i,j+1}\right| = -|a_2| \left|\theta^{i,j}\right| + |a_5| \left|\theta^{i,j+1}\right|$. According to Eq. 7.18 and after the simple manipulations we thus have

$$\sup_i \left|\theta^{i,j+1}\right| \leq 2 \sup_i \left|\theta^{i,j}\right| + C_1 \sup_{i,j} \left|\Phi_0^{i,j}\right|, \quad C_1 = h_0^2 \left(1 - \frac{1}{6k} + \frac{1}{k}\right)^{-1}. \tag{7.21}$$

In the same manner we can write the inequalities

$$\sup_i \left|\theta^{i,j}\right| \leq 2 \sup_i \left|\theta^{i,j-1}\right| + C_1 \sup_{i,j} \left|\Phi_0^{i,j}\right|,$$
$$\cdots$$
$$\sup_i \left|\theta^{i,1}\right| \leq 2 \sup_i \left|\theta^{i,0}\right| + C_1 \sup_{i,j} \left|\Phi_0^{i,j}\right|.$$

After the composition of all the inequalities, including the initial condition and the restriction $j \leq M$ we finally estimates

$$\sup_i \left|\theta^{i,j+1}\right| \leq 2^M (1 + C_1) \left(\sup_{i,j} \left|\Phi_0^{i,j}\right| + \sup_i \left|\Psi^i\right| \right), \quad i = 0, 1, \ldots, N. \tag{7.22}$$

It means that inequality (7.19) is valid for every $C \geq 2^M (1 + C_1)$ and, hence, the numerical scheme (7.18) is absolutely stable in the considered particular case $1/6 \leq k \leq 5/6$. Thus, according to the Philippov's theorem (e.g. see Godunov and Ryaben'kii 1987) the numerical solution converges to the exact solution of problem (7.1) and the order of its convergence coincides with the order of scheme approximation.

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