# 3D CRACKS GROWTH IN MATERIALS WITH GAS EMISSION IN BULK

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#### ABSTRACT

Three-dimensional problem on a slow quasi-stationary crack growth in materials exhibiting specific properties of gas emission in bulk is considered. The crack occupies arbitrary domain in plane in initial moment t. The connected diffusion-elasticity 3D problem is reduced to two 2D boundary integro-differential equations which then are solved numerically.

#### KEYWORDS

3D cracks, diffusion, cracks growth, gas emission in bulk, boundary integral equations.

#### INTRODUCTION

A number of materials used in modern engineering exhibit specific properties of gas emission in bulk under certain mechanical and/or physical influence or aging. Gas emission due to aging is typical for a number of polymers. Some metals and alloys applied in nuclear-power engineering become gas emissionable under radiation (Likhachev et al., 1982).

Gas emission in bulk can frequently cause crack or crack-like defects initiation and their kinetic propagation. In this case, crack kinetics analysis implies simultaneous consideration of gas diffusion into the crack and slow crack growth due to the action of inner gas pressure and other mechanical loads.

We suggest a numerical method for solving the 3D problem for a medium with cracks occupying a plane region. Problems of gas diffusion into crack and crack propagation are solved by reducing to integro-differential equations in the crack domain. The kinetics calculation is performed step by step procedure. The algorithms applied develop those suggested earlier (Balueva, 1993).

In model calculations, the crack velocity v at each point of the crack contour is assumed to be dependent on the stress intensity factor K at this point. The more general situation when v is a

functional of the gas concentration near the crack tip and stress intensity factor can be studied by a similar way. These results will be published elsewhere.

## STATEMENT OF THE PROBLEM

We consider the slow quasi-steady growth of a tensile crack initiated at t=0 and occupying a domain G in the plane  $x_3=0$ . The velocity v at each crack contour point is assumed to be dependent on the stress intensity factor N (as is adopted in kinetic crack theories) and specified by a curve v(N) which is the material function. The crack is growing under the action of a gas produced by gas emission sources distributed in bulk. The crack is modeled by an ideal sink (far from equilibrium state). The crack velocity is assumed to be small as compared to the transient period. Under this assumption, the flow into the crack can be found from the solution of the stationary diffusion problem for each t. Suppose that initially there are two diffusion sources of intensity W placed inside the body on the  $x_3$ -axis symmetrically at a distance  $\xi_3$  from the crack. In view of the symmetry with respect to the crack plane, we can consider the problem in the half-space  $x_3 \ge 0$ .

The boundary value problem for the gas concentration  $c(x_1, x_2)$  is following one:

$$\Delta c = -\frac{W}{D} \delta(x_1) \delta(x_2) \left[ \delta(x_3 - \xi_3) + \delta(x_3 + \xi_3) \right],$$

$$c \Big|_{x_3 = 0} = 0, \quad (x_1, x_2) \in G; \quad \frac{\partial c}{\partial x_3} \Big|_{x_3 = 0} = 0, (x_1, x_2) \notin G; c \Big|_{x_3 = \infty} = 0,$$
(1.1)

where D is the coefficient of gas diffusion in the medium.

The diffusion flow density  $q(x_1,x_2)=\partial\,c/\partial\,x_3\big|_{x^3=0}$  for  $(x_1,x_2)\in G$  is the unknown function in the problem. As usual, to construct an integral equation for q, we first consider the gas diffusion problem with sources in a medium without the crack:

$$\Delta c_o = -\frac{W}{D} \delta(x_1) \delta(x_2) [\delta(x_3 - \xi_3) + \delta(x_3 + \xi_3)], \tag{1.2}$$

$$\frac{\partial c_o}{\partial x_3}\Big|_{x_3=o}=0, \quad c_o\Big|_{x_3=\infty}=0$$

The solution to problem (1.2) is the function

$$c_{o}(x_{1}, x_{2}, x_{3}) = \frac{W}{4\pi D} \left(\frac{1}{R_{1}} + \frac{1}{R_{2}}\right), \text{ where}$$

$$R_{1,2} = \sqrt{x_{1}^{2} + x_{2}^{2} + (x_{3} \pm \xi_{3})^{2}}$$
(1.3)

and the gas concentration in the crack plane is given by

$$c_o(x_1, x_2, 0) = \frac{W}{2\pi D} \frac{1}{\sqrt{x_1^2 + x_2^2 + \xi_3^2}}.$$
 (1.4)

Let us now write out the solution to the diffusion problem without sources but with the gas concentration inside the crack to be equal in magnitude and opposite in sign to that in the first problem:

$$\Delta c = 0$$
,  $c|_{x_3=0} = -\frac{W}{2\pi D} \frac{1}{\sqrt{x_1^2 + x_2^2 + \xi_3^2}}, (x_1, x_2) \in G;$  (1.5)

$$\frac{\partial c_o}{\partial x_3}\Big|_{x_3=o}=0, \quad c_o\Big|_{x_3=o}=0.$$

The following integral equation is obtained for the diffusion flow density q from Eq.(1.5):

$$\Delta c = 0$$
,  $c|_{x_3=0} = -\frac{W}{2\pi D} \frac{1}{\sqrt{x_1^2 + x_2^2 + \xi_3^2}}, (x_1, x_2) \in G;$  (1.6)

Similarly, if a nonzero gas concentration  $c^o:c\Big|_{x_1=o}=c^o$ ,  $(x_1,x_2)\in G$  is given inside the crack, then we arrive at the integral equation

$$\frac{1}{2\pi} \iint_{G} \frac{q(\xi_{1},\xi_{2}) d\xi_{1} d\xi_{2}}{\sqrt{(x_{1}-\xi_{1})^{2}+(x_{2}-\xi_{2})^{2}}} = -\frac{W}{2\pi D} \frac{1}{\sqrt{x_{1}^{2}+x_{2}^{2}+\xi_{3}^{2}}}. \tag{1.7}$$

The following integral equation is valid if two sources symmetric with respect to the crack plane are placed at arbitrary points  $(a,b,\xi_3)$  and  $(a,b,-\xi_3)$  in bulk:

$$\frac{1}{2\pi} \iint_{G} \frac{q(\xi_{1}, \xi_{2}) d\xi_{1} d\xi_{2}}{\sqrt{(x_{1} - \xi_{1})^{2} + (x_{2} - \xi_{2})^{2}}} = \frac{W}{2\pi D} \frac{1}{\sqrt{x_{1}^{2} + x_{2}^{2} + \xi_{3}^{2}}} - c^{\circ}(x_{1}, x_{2}).$$
(1.8)

Using the superposition principle, we obtain the following equations for several point sources of gas diffusion inside the body or for those distributed with density  $W(x_1,x_2,x_3)$ :

$$\frac{1}{2\pi} \iint_{G} \frac{q(\xi_{1}, \xi_{2}) d\xi_{1} d\xi_{2}}{\sqrt{(x_{1} - \xi_{1})^{2} + (x_{2} - \xi_{2})^{2}}} = -\frac{W}{2\pi D} \frac{1}{\sqrt{x_{1}^{2} + x_{2}^{2} + \xi_{3}^{2}}}.$$
 (1.9)

$$\iint_{G} \frac{q(\xi_{1}, \xi_{2})d\xi_{1} d\xi_{2}}{\sqrt{(x_{1} - \xi_{1})^{2} + (x_{2} - \xi_{2})^{2}}} = \frac{1}{D} \sum_{i} \frac{W_{i}}{\sqrt{(x_{1} - a_{i})^{2} + (x_{2} - a_{i})^{2} + \xi_{3i}^{2}}},$$
(1.10)

where  $W_i$  are the intensities of the sources at the points  $(a_i,b_i,\pm\xi_{3i})$  and T is the region of diffusion sources distribution with density  $W(x_1,x_2,x_3)$ .

To search for the elastic fields induced by the gas diffusion into the crack, we consider the problem on a normal tensile crack with load p applied to its surfaces, where p is the gas pressure, which depends on the crack volume and mass of gas entered. The gas is assumed to be ideal; then the crack volume V, the mass of the gas V, and the pressure p are related by the Clapeyron equation V=MRT/ $\mu$ . Here  $\mu$ , V, and V are the molar mass of the gas, the gas

constant per mole, and absolute temperature, respectively. Reducing the elasticity problem to boundary integral equations, we obtain the system

$$\frac{1}{2\pi} \iint_{G} \frac{q(\xi_{1}, \xi_{2}) d\xi_{1} d\xi_{2}}{\sqrt{(x_{1} - \xi_{1})^{2} + (x_{2} - \xi_{2})^{2}}} = -\frac{W}{2\pi D} \frac{1}{\sqrt{x_{1}^{2} + x_{2}^{2} + \xi_{3}^{2}}}.$$
 (1.11)

$$\frac{W}{D} = \frac{1}{\sqrt{x_1^2 + x_2^2 + \xi_3^2}} = \iint_{G(t)} \frac{q(\xi_1, \xi_2) d\xi_1 d\xi_2}{\sqrt{(x_1 - \xi_1)^2 + (x_2 - \xi_2)^2}},$$
(1.12)

$$pV = nRT, (1.13)$$

$$V(t) = \iint_{G(t)} u(\xi_1, \xi_2) d\xi_1 d\xi_2, \tag{1.14}$$

$$V(t) = \iint_{C(t)} u(\xi_1, \xi_2) d\xi_1 d\xi_2, \tag{1.15}$$

$$n(t + \Delta t) = n(t) + Q\Delta t, \tag{1.16}$$

$$u(\xi, s, t) = \frac{4(1 - v^2)}{E} N(s, t) \sqrt{\xi}, \qquad (1.17)$$

$$v(s,t) = f(N(s,t)),$$
 (1.18)

$$R(t + \Delta t, s) = R(t, s) + v(t, s)\Delta t, \qquad (1.19)$$

where integral equation (1.11) for  $q(x_1,x_2)$  can be replaced by Eqs. (1.7)-(1.10) depending on the number of sources and their distribution. Equation (1.12) is the integro-differential equation for the crack surfaces displacement  $u(x_1,x_2)$ ; further,  $n,Q=\partial n/\partial t$ , E, and v are the number of gas moles in the crack, gas flow rate through the crack, Young's modules, and Poisson's ratio of the medium, respectively. Equations (1.17)-(1.19) provide the calculation of the stress intensity factor N and of the new crack contour.

The solution is performed stepwise (Balueva at al.,1992). The main computational difficulties of the first t-step are related to solving integro-differential equations (1.11)-(1.12) and in searching for a new crack contour via the calculated velocities v at the previous contour points (see Eq.(1.18)). The last computation is a separate calculational problem. A procedure for solving the elasticity problem for a normal tensile crack (Eq. (1.12)) has been developed (Goldstein at al., 1973). For this reason, we focus on a numerical method for solving the diffusion equation (1.11). In case of a circular crack region, we obtain an analytic solution.

## NUMERICAL METHOD FOR SOLVING THE DIFFUSION EQUATION

Our method for solving the integro-differential equation is based on the variational-difference method (Balueva et al., 1985). Namely, after discretization, the values of q at the grid points are searched for as an expansion through a system of coordinate functions  $\psi_{p1p2}$ ,

$$q(x_1, x_2) = \sum_{p1p2} c_{p1p2} v_{p1p2}(x_1, x_2, h), \qquad (2.1)$$

where  $\psi_{p1p2}$  is a bilinear spline function with a support in the four grid cells adjacent to the point  $(p_1h,p_2h)$  of the grid with the step h.

The coefficients  $c_{p_1p_2}$  coincide with the values of  $q(x_1,x_2)$  at the grid points and are found by minimizing the corresponding quadratic functional:

$$\min \left\{ I(h) = \sum_{p_1 p_2} \sum_{q_1 q_2} a_{p_1 - q_1, p_2 - q_2} c_{p_1 p_2} c_{q_1 q_2} + 2 \sum_{p_1 p_2} c_{p_1 p_2} b_{p_1 p_2} \right.$$
(2.2)

$$a_{p_1p_2q_1q_2} = a_{|p_1-q_1|,|p_2-q_2|} = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{1}{|\xi|} \psi_{p_1p_2}(\xi,h) \overline{\psi_{q_1q_2}(\xi,h)} d\xi, \qquad (2.3)$$

$$\psi_{p_{1}p_{2}}(\xi,h) = h^{2}e^{ih(p_{1}\xi_{1}+p_{2}\xi_{2})} \frac{sin^{2}\left(\frac{1}{2}h\xi_{1}\right)}{\left(\frac{1}{2}h\xi_{1}\right)^{2}} \frac{sin^{2}\left(\frac{1}{2}h\xi_{2}\right)}{\left(\frac{1}{2}h\xi_{2}\right)^{2}},$$
(2.4)

$$b_{p_1p_2} = \iint_{g^{2n}} p(x_1, x_2) \psi(x_1, x_2) dx_1 dx_2$$
 (2.5)

$$p(x_1, x_2) = \frac{W}{D} \frac{1}{\sqrt{x_1^2 + x_2^2 + \xi_3^2}}$$
 (2.6)

The minimization is carried out by the gradient projection method with an automatic step choice according to the relation between the linear and the actual functional increments.

## AXISYMMETRIC PROBLEM OF DIFFUSION FROM A POINT SOURCE

The integral equation (1.11) in the case of a circular crack of radius a and a point source lying on the  $x_3$ -axis acquires the form

$$\int\limits_0^{2\pi} d\phi \int\limits_0^a \frac{q(\rho)\rho d\rho}{\sqrt{r^2+\rho^2+2r\rho\cos\phi}} = g(r), \quad r \le a, \tag{3.1}$$

$$g(r) = \frac{W}{D} \frac{1}{\sqrt{r^2 + \xi_3^2}}$$

This integral equation (3.1) can be rewritten

$$\int_{0}^{a} q(\rho)K(\frac{2\sqrt{r\rho}}{r+\rho})\frac{\rho d\rho}{r+\rho} = \frac{1}{4}g(r), \tag{3.2}$$

$$K(k) = \int_{0}^{2\pi} \frac{d\phi}{\sqrt{1 - k^2 \sin^2 \phi}},$$
 (3.3)

where K(k) is the complete elliptic integral of the first kind

Using properties of Bessel functions, we have

$$\frac{2}{\pi} K \left( \frac{2\sqrt{r\rho}}{r+\rho} \right) \frac{1}{r+\rho} = \int_{0}^{2\pi} J_0(ur) J_0(u\rho) du, \tag{3.4}$$

and Eq. (3.2) becomes

$$\int_{0}^{\infty} J_{0}(ur) du \int_{0}^{a} q(\rho) \rho J_{0}(u\rho) d\rho = \frac{\pi}{8} g(r), \quad r \le a.$$
 (3.5)

Denote

$$\int_{0}^{a} q(\rho) \rho J_{0}(u\rho) d\rho = \Phi(u). \tag{3.6}$$

Then Eq. (3.5) can be represented in the form

$$\int_{0}^{\infty} \Phi(u) J_{0}(ur) du = \frac{1}{2\pi} g(r), \quad 0 \le r \le a.$$
 (3.7)

Using properties of the Bessel transformation, from Eq. (3.6) we obtain

$$\int_{0}^{\infty} \Phi(u)u J_{0}(ur) du = \begin{cases} g(r), & \text{for } r \leq a \\ 0, & \text{for } r > a \end{cases}$$
(3.8)

Thus, we arrive at the system of dual integral equations

$$\int\limits_0^\infty \Phi(u) J_0(ur) \, du = \frac{1}{\pi} g(r), \quad 0 \leq r \leq a,$$

$$\int_{0}^{\infty} u \Phi(u) J_{0}(ur) du = 0, \quad r > a.$$
 (3.9)

The solution to system (3.9) has form

$$\Phi(\mathbf{u}) = \frac{1}{\pi^2} \int_0^{\mathbf{a}} \cos \mathbf{u} t \left( \frac{\mathbf{d}}{\mathbf{d}t} \int_0^t \frac{y \mathbf{g}(\mathbf{y}) \, d\mathbf{y}}{\sqrt{t^2 - \mathbf{y}^2}} \right) d\mathbf{t}, \tag{3.10}$$

or after substituting of g(y)

$$\Phi(u) = \frac{1}{\pi^2} \frac{W}{D} \int_0^a \cos ut \left( \frac{d}{dt} \int_0^t \frac{y \, dy}{\sqrt{y^2 + c^2 \sqrt{t^2 - y^2}}} \right) dt,$$

from that we can find function q(r) in need by formula

 $q(r) = \int_{0}^{\infty} \Phi(u)u J_{0}(ur) du.$  (3.11)

Omitting cumbersome details of integration, let us write out the final expression for diffusion flux density through the crack

$$q(r) = \frac{1}{\pi} \frac{\xi_3}{\sqrt{(r^2 + \xi_3^2)^3}} + \frac{1}{\pi^2} \frac{\xi_3}{(r^2 + \xi_3^2)\sqrt{a^2 - r^2}} - \frac{1}{\pi^2} \frac{\xi_3}{\sqrt{(r^2 + \xi_3^2)^3}} \arctan \frac{\sqrt{a^2 - r^2}}{r^2 + \xi_3^2} (3.12)$$

As the crack radius  $a\rightarrow\infty$ , the solution has the asymptotics

$$q(r) \rightarrow \frac{1}{2\pi} \frac{\xi_3}{\sqrt{(r^2 + \xi_3^2)^3}}$$

This formula coincides with the solution to the problem on a diffusion source in a half-space. On the crack contour, that is, as  $r\rightarrow a$ , we have the asymptotics

$$q(r) \rightarrow \frac{1}{\pi^2} \frac{1}{(\xi_3 + a^2 / \xi_3) \sqrt{a^2 - r^2}}$$

Thus, this solution has a root singularity, which is actually observed in the problem of a gas diffusion into the crack for consideration given at infinity.

Comparison was made of numerical results with those obtained analytically. Good agreement is observed in the crack domain up to the last but one boundary node in the vicinity of the contour. The numerical solution becomes "bad" at the gird points adjacent to the boundary. This is due to the root singularity of solution on the crack contour. An effective Boundary Refinement Method is applied for improvement of numerical solution near boundary.

## CRACK PROPAGATION DUE TO GAS DIFFUSION FROM THE BULK SOURCES

Software is developed to calculate the crack propagation time and evolution of the crack shape and sizes under the action of gas diffusion from the unit source or sources distributed in bulk with a given density. These program is based on the described methods for solving the integrodifferential equations (1.11) of the diffusion problem and eqs.(1.12) of the elasticity problem. A quasi-steady statement of the problem is used. System (1.11)-(1.19) is solved at each time step. The incubation period  $t_i$  before the crack growth start is calculated. This is a time before the crack opening under the gas diffusion action achieves the value for which the maximum stress intensity factor along the crack contour becomes greater than the fracture toughness threshold value  $K_{sec}$ .

Calculation of the growth time  $t_m$  is performed by the following scheme:

- 1) the gas pressure is calculated in the current crack region G(t):  $p^2(t) = n(t)RT/V_1(t)$ , where  $V_1(t)$  is the volume of the crack occupying the new region G(t) for unit loading p=1, the gas mass n(t) being found at the previous step.
- 2) the stress intensity factor along the crack contour is calculated and used for calculation of the crack velocity  $\mathbf{v}_1$ .

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- 3) normal distances toward the crack contour overlapping discrete contour points during this propagation are defined as  $\Delta_i = v_i \Delta t$ . Time interval  $\Delta t$  is calculated so that contour points spreading with maximum velocity  $v_1$  pass a small distance  $\Delta u$  chosen experimentally.
- a new contour shape is defined using a smoothing procedure over propagating and stationary points coordinates.
- 5) the diffusion problem is solved; the integral flow  $q(x_1, x_2)$  through the crack surface, the total gas flow rate Q, and the new gas amount in the crack  $n(t + \Delta t) = n(t) + Q\Delta t$  are defined.
  - 6) the above procedure is repeated starting from step 1.

Model calculations were performed for a circular plane crack. Its kinetics was studied in the case of the gas diffusion from a unit bulk source. The incubation period  $t_i$  and time  $t_m$  of the crack growth from the initial to double radius were calculated. The dependence of the values  $t_i$  and  $t_m$  on the distance,  $\xi_3$ , from the diffusion source to the crack plane was studied. On diminishing the distance  $\xi_3$ , the gas flux to the crack increases and the gas pressure becomes greater, thus leading to the stress intensity factor growth along the contour. As a result, the velocity tends to its stationary value (on kinetic diagram), propagation and incubation times being practically independent of  $\xi_3$ . One more series of calculation was performed to study the dependence of life-time on the diffusion source intensity W. The greater the source intensity, the less is the life-time.

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