

# Corrosion Analysis using Non-linear Parabolic Equation

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*Abstract - Corrosion of zirconium and its alloys is of great interest due to the fact that these materials are used in the operation of nuclear energy installations, of great responsibility as they are working using special parameters. Mathematical modelling of physical phenomena was performed using partial derivative equations. Thus, for homogeneous environments (metal-zirconium) the second law of Fick has been used, and for the oxide layer - the non-linear parabolic equation specialized in modelling oxygen diffusion in porous media.*

**Index Terms-**Fick equations, Fokker equation, non-linear parabolic equation, linear combinations x-t method.

## I. INTRODUCTION

Many phenomena and processes of nature are modelled mathematically using equations with partial derivatives. Thus, in the beginnings of partial derivative equations, all mathematical problems analyzed, were linear. Subsequently, problems of differential geometry have given rise to non-linear partial derivative equations. The study of partial derivative equations has been encouraged and classic theory of variational calculation [5], [8]. The current paper relies on prior basic knowledge of the main differential operators, the definition of which we are presenting here [4], [10]:

(a) Gradient operator  $\nabla$  assigns a scalar field  $u$  of class  $C^1$  (continue and derivable) to a vector field, which is defined in Cartesian coordinates. Vector field  $\nabla u$  is directed, in the direction of the greatest increase in his  $u$ , in every point.

(b)  $Div v$  - divergence of a vector field is a scalar field. The notation  $u$  used in differential equations of mathematical physics actually represents a concentration  $c$ , commonly used in applications.

The diffusion is labelled with "a" in physical mathematics equations, respectively, with a "D", in practical applications. The current paper studies the corrosion models for "zircaloy-4". The name "zircaloy" denominates alloys with high content of zirconium, which is corrosion-resistant [1], [2], [3]. Also, various concentrations of niobium, chromium, nickel, thorium and others are added in very small quantities [1], [2], [4]: zircaloy-1, contains zirconium and 2.5% tin; in order to counteract the effect of corrosion and obtain better alloys other elements have been added: zircaloy-2 (Zyr-2), contains zirconium 98.25%, 1.45% tin, 0.10% chromium, 0.135 % iron, 0.055 % nickel, and 0.01 % hafnium. The alloy most commonly used for this purpose is: zircaloy-4 (Zry-4), containing zirconium 98.25 %, 1.45 % tin, 0.21 %

iron, 0.1 % chromium, and 0.01 % hafnium [2]. With the functioning of a nuclear reactor, the fuel is natural uranium which is burned in the "CANDU" reactor, using heavy water of nuclear purity as moderator and cooling agent. Fuel for this type of reactor is natural uranium in the form of uranium dioxide pellets enclosed in a sheath of an alloy of zirconium, by welding, closed at the ends [1], [3], [8]. Modelling corrosion involves a thorough knowledge of the evolution of oxygen concentration in space and time. The concentration of zirconium in zircaloy is very high, calculations taking in account only zirconium are common.

## II. PROBLEM FORMULATION

### A. Method of separation of variables

Fick's second law (also called the diffusion-convection law), or the equation of homogeneous parabolic diffusion is [9]:

$$\frac{\partial u}{\partial t} - a \frac{\partial^2 u}{\partial x^2} = c. \quad (1)$$

The  $u = u(x, t)$  represents the function at the given point  $x$  and at time  $t$ , and  $a$  is a positive constant. A general form of the parabolic equations modelling concentration variation in time and space  $c = c(x_i, t)$  is:



Which is a non-auto adjoint equation with the elliptical component [6]. Convective diffusion is modelled by Fokker-Planck equation. The solution of equation (1) is classically done through the use of three methods, which will be described as follows. The first method is the method of separation of variables and supposes that the solution to the problem  $u(x, t)$  is

$$u(x, t) = X(x)T(t), \quad (3)$$

Which in the final stage becomes



This form suggests that the solution is a series of functions converging uniformly

$$u(x, t) = \sum_{n=1}^{\infty} u_n(x, t) = \sum_{n=1}^{\infty} A_n \sin \frac{n\pi x}{l} e^{-\frac{n^2 \pi^2 a^2 t}{x^2}} \quad (5)$$

with the coefficient  $A_n$ :

$$A_n = \frac{2}{l} \int_0^l f(x) \sin \frac{n\pi x}{l} dx, \quad (6)$$

**B. Transformation method**

By applying this method, the Fourier transformation in relation to variable  $x$  is

$$\int_{-\infty}^{+\infty} u(x,t) e^{-i\lambda x} dx = \int_{-\infty}^{+\infty} \varphi(\lambda) e^{-i\lambda x} dx \quad (7)$$

After transformations, and in accordance with the inversion theorem, the following solution is obtained

$$u(x,t) = \frac{1}{2a\sqrt{\pi t}} \int_{-\infty}^{+\infty} u(\mu) e^{-\frac{(x-\mu)^2}{4a^2 t}} d\mu \quad (8)$$

also known as the Poisson equation

$$\Delta u = f(u) \quad (9)$$

and reaction-diffusion

$$u_t - \Delta u = f(u), \quad (10)$$

Equations that are semi-linear [5]

**C. Fourier integral method**

With this method, similarly to the Fourier transformation, the solution begins using the variable separation method and assuming that the solution to the problem  $u(x,t)$  is of the form (3), and

$$U(x,t) = X(x) T(t) = a^2 X(x) T(t). \quad (11)$$

We note

$$-\mathcal{L}^2 = \frac{X''}{X} = \frac{T'}{T} \quad (12)$$

and then integrate separately the two differential equations:

$$\begin{aligned} X'' + \lambda^2 X &= 0 \\ X &= C_1 \cos(\lambda x) + C_2 \sin(\lambda x) \end{aligned} \quad (13)$$

From the equation

$$T'' + a^2 \lambda^2 T = 0, \quad T = C e^{-a^2 \lambda^2 t} \quad (14)$$

with  $T$  and  $X$  calculated, replacing  $u(x,t)$  fourfold

$$u_\lambda(x,t) = e^{-a^2 \lambda^2 t} [A(\lambda) \cos(\lambda x) + B(\lambda) \sin(\lambda x)], \quad (15)$$

For each  $\lambda$  the solution  $u_\lambda(x,t)$  is obtained. The sum of solutions is a solution of the differential equation:

$$\begin{aligned} u(x,t) &= \sum_{\lambda} e^{-a^2 \lambda^2 t} [A(\lambda) \cos(\lambda x) + B(\lambda) \sin(\lambda x)] \\ u(x,t) &= \int_0^{\infty} e^{-a^2 \lambda^2 t} [A(\lambda) \cos(\lambda x) + B(\lambda) \sin(\lambda x)] d\lambda \\ u(x,0) &= \varphi(x) = \int_0^{\infty} [A(\lambda) \cos(\lambda x) + B(\lambda) \sin(\lambda x)] d\lambda \\ e^{-a^2 \lambda^2 t} &= 1, \end{aligned} \quad (16)$$

It is assumed that the function  $\varphi(x)$  can be written in the form of a Fourier integral:

$$\begin{aligned} \varphi(x) &= \frac{1}{\pi} \int_0^{\infty} \left( \int_{-\infty}^{+\infty} \varphi(x) \cos \lambda(\alpha - x) d\alpha \right) d\lambda \\ u(x,t) &= \frac{1}{\pi} \int_0^{\infty} \left[ \varphi(\alpha) \int_{-\infty}^{+\infty} e^{-a^2 \lambda^2 t} \cos \lambda(\alpha - x) d\lambda \right] d\alpha \end{aligned} \quad (17)$$

By identification, the resulting coefficients are:

$$\begin{aligned} A(\lambda) &= \frac{1}{\pi} \int_{-\infty}^{+\infty} \varphi(\alpha) \cos(\lambda(\alpha - x)) d\alpha \\ B(\lambda) &= \frac{1}{\pi} \int_{-\infty}^{+\infty} \varphi(\alpha) \sin(\lambda(\alpha - x)) d\alpha \end{aligned} \quad (18)$$

and the solution

$$u(x,t) = \frac{1}{\pi} \int_0^{\infty} e^{-a^2 \lambda^2 t} \left( \int_{-\infty}^{+\infty} \varphi(x) \cos(\lambda(\alpha - x)) d\alpha \right) d\lambda \quad (19)$$

Reversing the order of integration, let us calculate the integral

$$\begin{aligned} \int_0^{\infty} e^{-a^2 \lambda^2 t} \cos(\lambda(\alpha - x)) \pi d\lambda &= \\ = \frac{1}{a\sqrt{t}} \int_0^{\infty} e^{-z^2} \cos(\beta z) dz \end{aligned} \quad (20)$$

in which

$$d\lambda = \frac{dz}{a\sqrt{t}} \quad (21)$$

Let us make the substitutions:

$$a\lambda\sqrt{t} = z, \quad \lambda = \frac{z}{a\sqrt{t}} \Rightarrow d\lambda = \frac{dz}{a\sqrt{t}} \quad (22)$$

$$\lambda(\alpha - x) = \frac{z(\alpha - x)}{a\sqrt{t}} = \beta$$

and with notations:

$$\beta = \left( \frac{\alpha - x}{\alpha \sqrt{t}} \right), \quad K(\beta) = \int_0^{\infty} e^{-z^2} \cos \beta z dz, \quad (23)$$

$$K'(\beta) = -\int_0^{\infty} e^{-z^2} z \sin \beta z dz.$$

Integrating by parts:

$$K'(\beta) = \frac{1}{2} [e^{-z^2} \sin \beta z]_0^{\infty} - \int_0^{\infty} \frac{\beta}{2} [e^{-z^2} \cos \beta z] dz$$

$$K'(\beta) = -\frac{\beta}{2} K(\beta), \quad K(\beta) = C e^{-\left(\frac{\beta}{2}\right)^2} \quad (24)$$

$$K(0) = \frac{\sqrt{\pi}}{2}, \quad K(\beta) = \frac{\sqrt{\pi}}{2} e^{-\frac{\beta^2}{4}}$$

Considering that

$$\int_0^{\infty} e^{-z^2 \lambda^2 t} \cos(\lambda(\alpha - x)) d\lambda = \frac{\sqrt{\pi}}{2\alpha\sqrt{t}} e^{-\frac{\beta^2}{4}} = \frac{\sqrt{\pi}}{2\alpha\sqrt{t}} e^{-\frac{(\alpha-x)^2}{4\alpha^2 t}} \quad (25)$$

we find the solution [5], [6]

$$u(x, t) = \frac{1}{2\alpha\sqrt{\pi t}} \int_{-\infty}^{+\infty} \varphi(x) e^{-\frac{(\alpha-x)^2}{4\alpha^2 t}} d\alpha \quad (26)$$

which is the solution to Fick's equation in the integral Poisson form, which can be calculated by this method.

Based on the Poisson equation (8) with variable  $\alpha$ , and if the function  $u_0(x)$  is odd

$$u_0(-x) = -u_0(x), \quad (27)$$

then we can rewrite:

$$u(x, t) = \frac{1}{2\alpha\sqrt{\pi t}} \int_{-\infty}^{+\infty} u_0(\mu) \left[ e^{-\frac{(x-\mu)^2}{4\alpha^2 t}} - e^{-\frac{(x+\mu)^2}{4\alpha^2 t}} \right] d\mu, \quad (28)$$

Making variable substitutions:

$$\alpha = \frac{(x-\mu)}{2at} \quad \text{and} \quad \beta = \frac{(x+\mu)}{2at}, \quad (29)$$

we find the solution

$$u(x, t) = \frac{u_0}{\sqrt{\pi}} \left\{ \int_{-\frac{x}{2\alpha\sqrt{t}}}^{\infty} e^{-\alpha^2} d\alpha - \int_{\frac{x}{2\alpha\sqrt{t}}}^{\infty} e^{-\beta^2} d\beta \right\} =$$

$$= \frac{u_0}{\sqrt{\pi}} \int_{-\frac{x}{2\alpha\sqrt{t}}}^{+\frac{x}{2\alpha\sqrt{t}}} e^{-\alpha^2} d\alpha = 2 \frac{u_0}{\sqrt{\pi}} \int_0^{+\frac{x}{2\alpha\sqrt{t}}} e^{-\alpha^2} d\alpha, \quad (30)$$

or, because it is more convenient, for small values of  $x$ , which is the case of the thickness of the layer of oxides, the following relation is used

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\alpha^2} d\alpha \quad (31)$$

The final solution is

$$u(x, t) = u_0 \text{erf} \left( \frac{x}{2\alpha\sqrt{t}} \right) \quad (32)$$

### III. SOLVING THE FIRST NON-LINEAR PARABOLIC EQUATION

#### A. Solving the non-linear parabolic equation, with the definition of flux as starting point

Due to physics considerations, based on the definition of flow, which is the first law of Fick

$$J = -D^* \frac{\partial c}{\partial x}, \quad [\text{mol}/\text{m}^2\text{s}], \quad (33)$$

where,  $c$  is the concentration, expressed in  $[\text{mol}/\text{m}^3]$ ,  $t$  is the time, expressed in  $[\text{s}]$ ,  $x$  is the distance, expressed in  $[\text{cm}]$ , and  $D^*$  is the coefficient of diffusion, expressed in  $[\text{cm}^2/\text{s}]$ . For the conservation of mass. Let us derivate once again the equation (33), resulting in

$$\frac{\partial c}{\partial t} + \text{div} J = 0, \quad \frac{\partial c}{\partial t} = -\text{div} J = -\text{div} \left( D^* \frac{\partial c}{\partial x} \right) \quad (34)$$

or taking the first and the last term

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x} \left( D^* \frac{\partial c}{\partial x} \right) \quad (35)$$

Expressing the  $D^* = \varphi(x) D$ , and  $\varphi(x)$  as a function of length, in which  $x$  can be a feature of the system, and  $D$  remains constant, then the result this equation with partial derivative, used for modelling this phenomenon of corrosion

$$\frac{\partial c}{\partial t} = D \frac{\partial}{\partial x} \left( \varphi(x) \frac{\partial c}{\partial x} \right) \quad (36)$$

or,

$$\frac{\partial c}{\partial t} = \text{div} (D \varphi(x) \text{grad}(c)) \quad (37)$$

The equation (37) is a non-linear parabolic equation, with elliptic component, somewhat atypical and creates serious problems for solving.

**B. Solving non-linear parabolic equation, with the Planck-Nernst diffusion equation as starting point**

The same result is reached starting from the relation that controls the diffusion of oxygen through layers of rust (oxides), called Planck-Nernst relation

$$J_i = -D_i \nabla c_i + \frac{D_i q_i}{k_B T} \nabla \phi \quad (38)$$

where  $J_i$  is the flow of species  $i$ ,  $c_i$  is the concentration of species  $i$ ,  $\phi$  is electrostatic potential, the  $D_i$  is the diffusion,  $q_i$  represents electric charge,  $e$  is the elementary charge of electron equal to approximately  $1.602 \times 10^{-19}$  C,  $k_B$  is Boltzmann's constant equal to approximately  $1.380 \times 10^{-23}$  J/K, and  $T$  is absolute temperature on a Kelvin scale.

If  $S_k$  is a source which consumes or releases oxygen, mass equilibrium is written

$$S_k = \frac{\partial c_k}{\partial t} + \nabla \cdot J_k \quad (39)$$

Considering  $S_k = 0$ , then the relation becomes

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \left( -D_i \nabla c_i + \frac{D_i q_i}{k_B T} \nabla \phi \right) \quad (40)$$

and, by not taking into account the term containing temperature, we obtain

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial x} (D_i \nabla c_i) \quad (41)$$

If  $D_i$  is proportional to  $D$  by a function of  $x$ , it follows the equation (36). For  $\varphi(x)=1$ , in the equation (2) Fick's law given by the equation (1) is obtained. A general form of parabolic equations used in modelling concentration variation in time and space is the form (2). In the following paragraph, two new methods used to obtain solution to equation (2) are presented.

**IV. SOLVING THE SECOND NON-LINEAR PARABOLIC EQUATION**

**A. First method**

Let us consider that the solution is a linear combination between the two parameters, the distance ( $x$ ) and time ( $t$ ). Derivatives of solution  $u(x,t)$  are:

$$\frac{\partial u}{\partial x} = \frac{du}{dy} \frac{dy}{d\alpha} \quad (42)$$

$$\frac{\partial u}{\partial t} = \frac{du}{dy} \frac{dy}{d\alpha} \quad (43)$$

Noting  $p$  and  $q$  coefficients linear combination of  $x$  and  $t$ , differential equation becomes

$$\frac{d^2 u}{dy^2} + \left( \frac{p}{f p^2} + \frac{q}{D f p^2} \right) \frac{du}{dx} = 0 \quad (44)$$

Also, noting:

$$F(x) = \left( \frac{p}{f p^2} + \frac{q}{D f p^2} \right), \quad \frac{du}{dy} = z \quad (45)$$

$$\frac{dz}{dy} + F(x)z = 0$$

and by separating the variables and integrating

$$z = K_1 e^{-F(x)y} \quad (46)$$

Coming back to the notation  $z$

$$\frac{du}{dy} = z = K_1 e^{-F(x)y} \quad (47)$$

The final solution is

$$u(x, t) = K_1 \frac{-1}{F(x)} e^{-yF(x)} + K_2 \quad (48)$$

Which represents the original solution of non-linear parabolic equation. Let us note that application of the method depends on the determination of the integration constants  $K_1$  and  $K_2$  and the pair of parameters  $p$ ,  $q$ ,  $y=px+qt$ . A new method for obtaining the solution for non-linear parabolic equation

$$\frac{\partial u}{\partial t} = D \left( \varphi(x) \frac{\partial^2 u}{\partial x^2} \right) \quad (49)$$

**B. The second method**

This method is subjected to the following conditions

$$\varphi(x) > 0 \text{ for } x > 0, \varphi(x) \in C^1, \varphi(x) = e^{-x} \quad (50)$$

The derivative is

$$D^{-1} u_t = \varphi'(x) u_x + \varphi(x) u_{xx} \quad (51)$$

For a uniform mathematical notation, we use the notations:

$$\varphi(x) = g(x), \quad \varphi'(x) = h(x) \quad (52)$$

The equation becomes

$$D^{-1} u_t = h(x) u_x + g(x) u_{xx} \quad (53)$$

Looking for a solution of the form

$$u(x,t) = v(x) + w(t), \quad (54)$$

with:

$$u_t = w', \quad u_x = v'(x), \quad u_{xx} = v''(x) \quad (55)$$

The equation can be solved if  $w'(t)=k$ , where  $k \in \mathbb{R}$ , and if it is divided into two equations:

$$w'(t) = k \tag{56}$$

and then calculate (59), from which:

$$g(x)v''(x) + h(x)v'(x) = kD^{-1}, \tag{57}$$

$$v'(x) = \omega(x), v(x) = \int_0^x \omega(\tau) d\tau + C, \tag{68}$$

the equation (57), as being an ordinary, linear differential equation.

The final solution is

By integrating the equation (56), we obtain  $w(t)$

$$u(x, t) = \frac{k}{D} \int_0^x \frac{C_2 + \tau}{g(x)} d\tau + C_3 + (kt + \lambda) \tag{69}$$

$$w(t) \in S_1 = \{kt = \lambda, k, \lambda \in \mathbb{R}\} \tag{58}$$

Its solving method is limited by the variation of parameter  $t$  (time) to a first-degree polynomial form

Let us resume solving equation, using notations

$$v'(x) = \omega(x) \tag{59}$$

$$w(t) = kt + \lambda, w'(t) = k, u(x, t) = v(x) + w(t), \tag{70}$$

and transforming the degree two equation (57) to the degree one equation

this being the second original solution.

The general form of the Fokker-Planck equation is

$$g(x) \omega'(x) + h(x)\omega(x) - kD^{-1} = 0 \tag{60}$$



$$- a(x,t)c(x,t)=f(x,t), \tag{71}$$

Let us solve the homogeneous equation

which includes a perturbation factor and a source. By applying for  $u(x, t)=c(x, t)$  concentrations, the equation has the simplified form

$$\frac{\dot{\alpha}(x)}{g(x)} = \frac{h(x)}{g(x)} \alpha(x) \Rightarrow \frac{\dot{\alpha}(x)}{\alpha(x)} = \frac{h(x)}{g(x)}, \tag{61}$$

equation which is derived a logarithm



$$[\ln \alpha(x)]' = \left[ \frac{h(x)}{g(x)} \right] \tag{62}$$

After integration

If  $D=D_2$  is diffusion, and  $D_1=D_1(x)$  a distance, by derivation, a speed  $v$  is obtained

$$\ln \alpha(x) = \int \frac{h(x)}{g(x)} dx + C, \tag{63}$$



where  $C$  is a constant of integration.

The solution of the logarithmic equation is

As a novelty, the term  $\partial u / \partial t$  is multiplied by a coefficient  $R$ , which is called delay coefficient. It may have a supraunitary impact value or a sub unitary one, and may delay or accelerate the diffusion process. As a result, Fokker partial differential equation becomes

$$\alpha(x) = \frac{C}{g(x)}, \tag{64}$$

$$R \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} - v \frac{\partial u}{\partial t}, \tag{74}$$

which is a general solution of ordinary differential equations of the type

To solve the Fokker equation, we are proposing an original method. Let  $y=y(x, t)$  and  $u=u(y)$ ,

$$\frac{dy}{dx} + P(x)y = Q(x), \tag{65}$$

Then, partial derivatives are:

with the homogeneous solution

$$\frac{\partial u}{\partial t} = \frac{du}{dy} \frac{\partial y}{\partial t}, \frac{\partial u}{\partial x} = \frac{du}{dy} \frac{\partial y}{\partial x}, \frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} \right) \tag{75}$$

$$y(x) = \frac{e^{-\int P(x) dx}}{g(x)} \left( C - \int_0^x Q(x) e^{-\int P(x) dx} dx \right), \tag{66}$$

These partial derivatives exist if variables are  $x$ , distance, and  $t$ , time, are independent of one another. By applying the Fourier method, the solution is a linear combination of  $x$  and  $t$ . The differential equation becomes

By identification, we obtain:



$$y = \omega(x), P(x) = \frac{h(x)}{g(x)}, Q(x) = -\frac{k}{D g(x)} \tag{67}$$



Let us note:

$$\frac{dw}{dy} = \frac{Rd}{K_1 D} \quad (77)$$

$$\frac{dz}{z} = \frac{v}{K_1} dy, \quad z = K_1 e^{\theta y}, \text{ and} \quad (78)$$

$$\frac{du}{dy} = K_1 e^{\theta y} \Rightarrow du = K_1 e^{\theta y} dy.$$

By integrating, the final solution is

$$u(x, t) = K_1 \frac{1}{\theta(D, R, x, t, v, p, q)} e^{y\theta(D, R, x, t, v, p, q)} + K_2, \quad (79)$$

with variables  $x, t$  and the parameters  $p$  and  $q$ .

This represents the original equation solution Fokker. In the literature, the solution is determined using the *erf* integral. Note that there is a certain resemblance between the convective diffusion equation (Fokker-Planck) and non-linear parabolic equation, as well as between the non-linear parabolic equation and Fick's Equation.

### V. NUMERICAL RESULTS

For the following numeric application, we have used the first original solution, since it has greater generalization. In the homogenous domain, i.e. - metal oxide, we applied Fick's second law in the following conditions [1]:  $c_0 = 500$  is the oxygen concentration at the interface oxide-metal (expressed in  $[\text{mg}/\text{cm}^3]$ );  $c_f = 0.01$  is final concentration, which tends towards zero  $t = 10^{14}[\text{s}]$ . At  $t = 10^{14}$  assumed only for testing the equation,  $x = 0.10 [\text{cm}]$  and  $D = 1.9 \times 10^{-14}$  is the diffusion coefficient (expressed in  $[\text{cm}^2/\text{s}]$ ). With the solution to the differential equation in the form:

$$c(x) = c_0 - (c_0 - c_f) \text{erfc} \left( \frac{x}{2\sqrt{Dt}} \right), \quad (D = a^2), \quad (80)$$

the following plot (Fig.1) is obtained. In the layer of black zirconium oxide, we have used:  $c_0 = 2600$  is the value of the oxygen concentration at the oxide interface-air (expressed in  $\text{mg}/\text{cm}^3$ );  $c_1 = 1500$  is the value of the oxygen concentration at the interface oxide-metal (expressed in  $[\text{mg}/\text{cm}^3]$ );  $D = 1.9 \times 10^{-9}$  is the diffusion coefficient (expressed in  $[\text{cm}^2/\text{s}]$ );  $v = 1.8 \times 10^{-6}$  is the speed of oxidation (expressed in  $[\text{cm}/\text{s}]$ );  $K_1 = -0.159$  is constant of integration;  $x = 50 \times 10^{-4}$ , oxide layer (expressed in  $[\text{cm}]$ );  $K_2 = 1.225 \times 10^3$  is constant of integration;  $t = 2.79 \times 10^3$  (given by the ratio  $x/v$ ). The solution to equation (36) is represented in 2-D and 3-D (Fig.2 and Fig.3). Difference between  $c_0 - c_1$ , represents the drop in concentration at the interface oxide-metal (Fig.2)

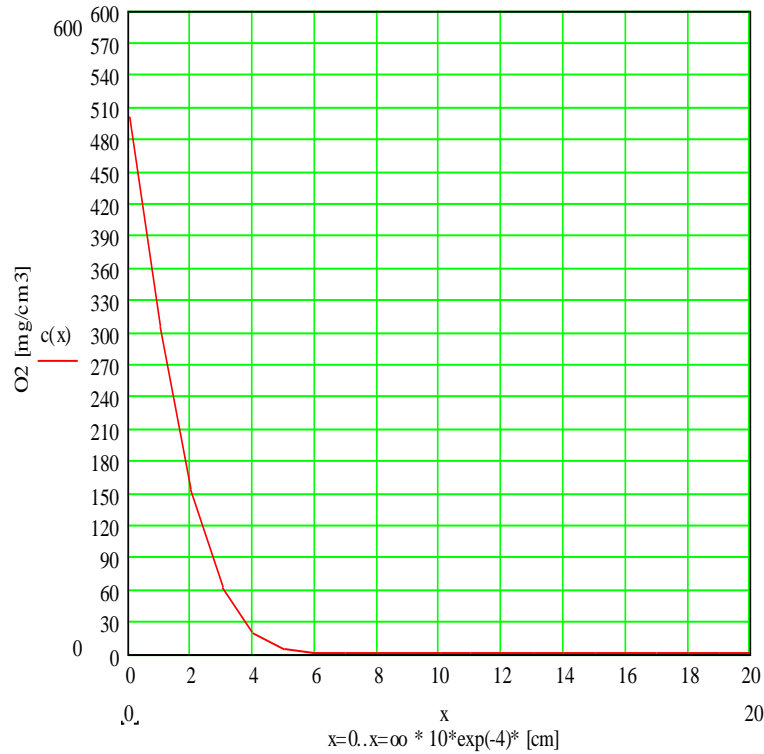


Fig.1. Changes in the concentration of oxygen in the metal:  $c_0 = 500, c_f = 0 [\text{mg}/\text{cm}^3], x [\text{cm}]$  - metal layer.

$$\frac{d}{dx} \left[ \frac{dc}{dx} \right] = \frac{v}{D} c \quad (81)$$

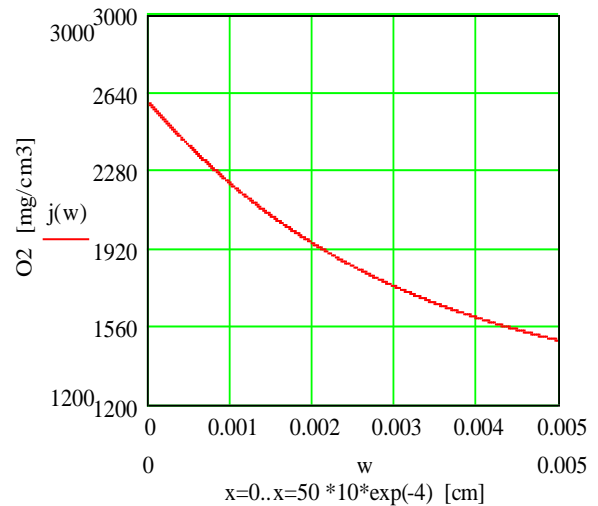
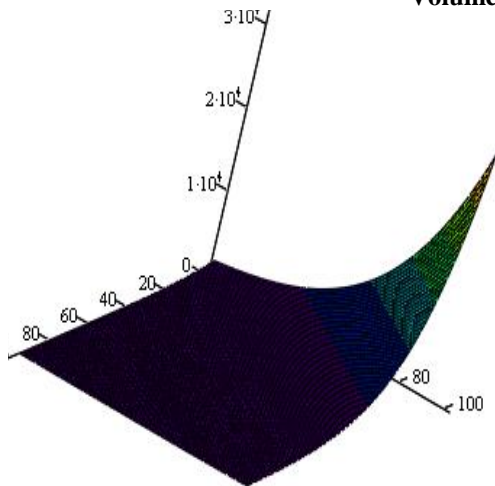


Fig.2. Changes in the concentration of oxygen in the layer of black zirconium oxide from  $c_0 = 2600.00$  to  $c_1 = 1499.90$  ( $\sim 1500.00$ )  $[\text{mg}/\text{cm}^3]$ .



**Fig.3.** Changes in the concentration of oxygen in the oxide layer of zirconium in black 3-D obtained with the data from Figure 2.

Let us do the transformation of the Fokker equation into the equation Fick through a linear combination between the variables  $x, t$  and two parameters  $p$  and  $q$ . Consider the following:  $c_2=c_0=2600$  represents initial concentration (expressed in  $[mg/cm^3]$ ),  $c_f=c_1=1500$  is final concentration,  $D=1.13 \times 10^{-9} [cm^2/s]$ ,  $x=0...50 \times 10^{-4} [cm]$  represents the distance,  $v=1.82 \times 10^{-6} [cm/s]$  is the speed, the constants  $p=v/(2D)=796.46$ , and the time  $t=(5010)v[s]$ .  
 $q = Dp^2 + pv = 2.15 \times 10^{-3}$

Fick's equation

$$FK(x) := \left[ c_f + (c_2 - c_f) \cdot \operatorname{erfc} \left[ \frac{x \cdot 10^{-4}}{\sqrt{4 \cdot D \cdot \left( \frac{x}{v} \cdot 10^{-4} \right)}} \right] \cdot 1 \right] \cdot 1 \quad (82)$$

is represented in Fig.4 with dotted line.

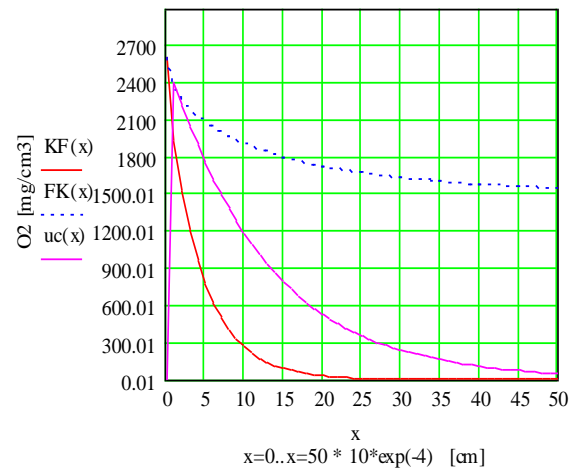
Fokker equation, after previous calculations

$$KF(x) := \left[ c_f + (c_2 - c_f) \cdot \operatorname{erfc} \left[ \frac{x \cdot 10^{-4}}{\sqrt{4 \cdot D \cdot \left( \frac{x}{v} \cdot 10^{-4} \right)}} \right] \cdot 1 \right] \cdot e^{-\left[ p \cdot x \cdot 10^{-4} + q \cdot \left( \frac{x}{v} \cdot 10^{-4} \right) \right]} \quad (83)$$

is represented in Fig.4 with continuous line. The solution obtained by integration

$$uc(x) := c_2 \cdot 1 \cdot \operatorname{erf} \left[ \frac{x}{\sqrt{4 \cdot D \cdot \left( \frac{x}{v} \cdot 10^{-4} \right)}} \right] \cdot e^{-\left( p \cdot x \cdot 10^{-4} + \frac{q}{v} \cdot x \cdot 10^{-4} \right)} \quad (84)$$

is represented in Fig.4 dashed line. Note that the ratio of proportionality between the two solutions Fokker and Fick, is the exponential of the linear combination on which it determinations have ben done. The method can be used for the Fokker equation with multiple variables.



**Fig.4.** The representation of solutions Fokker-Planck and Fick for  $x [cm]$ ,  $KF(x)$ ,  $FK(x)$ ,  $uc(x)$ .

## VI. CONCLUSIONS

The non-auto ad joint parabolic equation with elliptical component is used in modelling diffusion of oxygen in the process of corrosion. Another option would be using Fokker-Planck equation, but this equation differs from Fick equation by the term  $-v(du/dx)$ . We have transformed the Fokker-Planck equation to the Fick equation, choosing from the very beginning an analytical solution using differential equations with partial derivatives, specialized in modelling the diffusion of oxygen, such as the non-autoadjoint parabolic equation with elliptical component. The difficulty of mathematical calculations resided in determining the integration constants  $K_1 = -0.159$  and  $K_2 = 1.225 \times 10^3$  and the two variables  $p=107$  and  $q=15$ . Other data have been taken from experimental measurements. Also, it has been demonstrated that at least one of parameters  $p$  or  $q$  is comparable to the absolute value of the diffusion  $D$ , between  $10^{-5}$  and  $10^{-12}$ . It has also been showed that the solution to the differential parabolic equation, through the demonstration carried out, under certain conditions, it is a multiple of a linear combination of  $x, t, p$  and  $q$ .

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