Mathematical Modelling and Analysis
Volume 6 Number 1, 2001, pages 77–84

UNIQUENESS AND CONVERGENCE OF THE ANALYTICAL SOLUTION OF NONLINEAR DIFFUSION EQUATION

A.J. JANAVIČIUS, P. NORGĖLA and D. JURGAITIS

Šiauliai University

P. Višinskio 25, 5400 Šiauliai, Lithuania

E-mail: `AYanavi@takas.lt`

Received December 7, 2000; revised February 11, 2001

ABSTRACT

We have discussed the problems of uniqueness of the physical solution of the nonlinear diffusion equation. Here are considered two different ways to express the solutions in the power series. In the first case we will use the power-series expansion about the zero point. The accuracy of the obtained physical solution is evaluated. However, in this case we get an infinity of different solutions and the problem of the choice of the unique physical solution is considered using the expansion about the point of maximum penetration of the impurities. Then we get only two solutions which differ one from other only in the directions of the diffusion.

1. INTRODUCTION

The classical linear diffusion equation is derived from the Fokker-Planck equation. This linear diffusion equation is obtained by assuming that process is slow. We see that fitting an experimental profile tail region of impurities to classical $erfc(x/2\sqrt{Dt})$ tail region, where linear diffusion must occur with large velocity, is physicaly non acceptable. From the Braunian movement or random walkers theory the mean-square displacement $\sqrt{2Dt}$ must be approximately equal to the maximum penetration depth obtained from the nonlinear equation solution. The theoretically obtained profiles and maximum penetration depths of the impurities can be used for planar transistor formation only when the solutions of nonlinear diffusion equation are found uniquely.

In paper [1] the nonlinear diffusion equation

$$\frac{\partial}{\partial t}N = D_n\frac{\partial}{\partial x}\left(N\frac{\partial N}{\partial x}\right), \qquad (1.1)$$

where the diffusion coefficient and the current density were directly proportional to the concentration of impurities

$$D(t,N) = D_nN(x,t), \qquad (1.2)$$

was solved introducing the similarity variable

$$\xi = \frac{x}{\sqrt{D_st}}, \quad D_s = D_nN_s, \quad N_s = const. \qquad (1.3)$$

The obtained solution [1] was fitted with the experiment and it was compared the complementary error function. But in this paper we got more solutions with different depths of penetration. Therefore it founds the conditions and a method for the selection of the unique solution. The presented method can be useful for solving of the similar nonlinear diffusion equations [2], [3]. It can be used for describing of clouds and diffusion in dynamical systems where interactions between the particles are included.

2. THE EXPANSION OF THE SOLUTIONS IN THE POWER SERIES AT THE ORIGIN

Now we will consider the solutions of nonlinear diffusion equation (1.1) with the following boundary

$$N(0,t) = N_s, \quad N(\infty,t) = 0 \qquad (2.1)$$

and initial

$$N(x,0) = 0, \quad x > 0 \qquad (2.2)$$

conditions. Solution of equation (1.1) with conditions (2.1), (2.2) we must divide in two parts. It is possible to solve this problem by dividing it in to two parts. For the first part of problem (1.1)

$$\frac{\partial N}{\partial t} - D_n\frac{\partial}{\partial x}\left(N\frac{\partial N}{\partial x}\right) = 0, \quad t > 0, \quad x \in (0, x_0(t)), \qquad (2.3)$$

we must find the solutions which satisfies the conditions

$$N(0,t) = N_s, \quad N(x_0(t),t) = 0, \quad t > 0, \quad x_0(0) = 0. \qquad (2.4)$$

For the second part of problem

$$\frac{\partial N}{\partial t} - D_n \frac{\partial}{\partial x}\left(N\frac{\partial N}{\partial x}\right) = 0, \quad t > 0, \quad x_0(0), \tag{2.5}$$

we must get the solutions which satisfies the following conditions

$$N(\infty, t) = 0, \quad N(x_0(t), t) = 0, \quad t > 0, \quad N(x, 0) = 0, \quad x > 0. \tag{2.6}$$

For the second part of problem (2.5), (2.6) we have only trivial solution and we will consider only solution of first part of problem (2.3), (2.4).

Introducing the similarity variable (1.3) into the equation (2.3) we obtain the following nonlinear equation

$$2\frac{d}{d\xi}\left(f\frac{d}{d\xi}f\right) + \xi\frac{d}{d\xi}f = 0, \quad N(x,t) = N_s f(\xi); \quad \xi \in (0, \xi_0). \tag{2.7}$$

We can expand the solution of the last equation in the power series

$$f(\xi) = \sum_{n=0}^{\infty} a_n \xi^n, \tag{2.8}$$

with the following boundary conditions

$$f(0) = 1, \quad f(\xi_0) = 0. \tag{2.9}$$

The solution (2.8) we present like the family of one-parametrical solutions.

Substituting (2.8) into (2.3) we obtained the system of equations

$$2\sum_{m=0}^{\infty} b_{nm} + 2\sum_{m=0}^{\infty} c_{nm} + n a_n = 0,$$

$$b_{nm} = (n+1-m)(m+1)a_{n+1-m}a_{m+1}, \tag{2.10}$$

$$c_{nm} = (n+2-m)(n+1-m)a_{n+2-m}a_m, \quad n = 0, 1, 2, ...$$

As an example we can write the first six equations

$$2(a_1)^2 + 4a_2a_0 = 0,$$

$$12a_1a_2 + 12a_0a_3 + a_1 = 0,$$

$$24a_1a_3 + 24a_0a_4 + 12(a_2)^2 + 2a_2 = 0,$$

$$40a_1a_4 + 40a_2a_3 + 40a_0a_5 + 3a_3 = 0, \tag{2.11}$$

$$60a_1a_5 + 60a_2a_4 + 30(a_3)^2 + 60a_0a_6 + 4a_4 = 0,$$

$$84a_1a_6 + 84a_2a_5 + 84a_3a_4 + 84a_0a_7 + 5a_5 = 0.$$

Solving the system of six equations (2.11), we can find the six unknown coefficients of truncated expansion (2.8) only taking $a_7 = 0$. From the boundary condition at the zero point $f(0) = 1$ we get $a_0 = 1$. On the frontier of diffusion we must require $f(\xi_{06}) = 0$. The less exact solutions [1] of equation (2.3) were obtained in the form of polynomials [1] after truncation of expansion (2.8). The accuracy of these solutions can be evaluated by the size of the last terms $a_n(\xi_{0n})^n$ of the polynomials. From [1] we get $a_4(\xi_{04})^4 = 0,0024$, $a_5(\xi_{05})^5 = 0,00024$. The maximum value of function $f(\xi)$ at the origin $f(0) = 1$ is much larger and terms $a_n\xi^n$ for $n > 4$ in the power series (2.8) can be truncated. The polynomials where terms with $n \geq 4$ are included practically coincide. For n equations (2.10) we have $n+1$ unknown coefficients a_n. It is a consequence of the fact that the boundary condition $f(\xi_0) = 0$ is not included in the series (2.8). In this case by increasing the number of equations in the truncation of the original system (2.10) we get more solutions. Then we have a group of solutions which satisfies the condition $f(\xi_0) = 0$ and nonphysical solutions which do not satisfy this boundary condition. The obtained solutions of truncated system (2.10) are presented in the Table 1 [4]. We have not only one physical solution expressed in the polynomials of power n. Taking into account random walking theory [5] and (1.3), we got $\xi_0 = \sqrt{2}$. Then in [1] we choose $\xi_{05} = 1,617$ and the explanation of this difference has been presented. If we use (2.4), the following symmetry of the function can be obtained

$$f(-\xi) = \sum_{n=0}^{\infty}(-1)^n a_n \xi^n. \tag{2.12}$$

If coefficients a_n in the system (2.11) are changed by $(-1)^n a_n$, we get coefficients $(-1)^n a_n$ which also satisfy this system. Then from the last result we find out that for the zeros $\xi_{0n,i}$ of function $f(\xi)$ we have the zeros $-\xi_{0n,i}$ of function $f(-\xi)$ which is also the solution of the equation (2.3). The index $0n,i$ for ξ signifies i-th zero of i-th solution for n-th order polynomial. For $n = 8$ we got two more solutions with following meanings of the zeros $\xi_{08,2} = 3,27$, $\xi_{08,3} = 4,27$. The coefficients of the obtained solutions are presented in Table 1 [4]. The two last solutions are not exact and represent the nonrealistical penetrations depths. Solving the system (2.10) for seven and eight equations we got the following set of the zeros

$$\xi_{07,1} = 1,6167,\ \xi_{08,1} = 1,6161,\ \xi_{07,2} = 3,65,$$
$$\xi_{08,2} = 3,27,\ \xi_{07,3} = 4,46,\ \xi_{08,3} = 4,27. \tag{2.13}$$

The accuracy of those approximate solutions can be evaluated by the terms

$$a_{8,1}(\xi_{08,1})^8 = 7,9 \cdot 10^{-7}, \quad a_{8,2}(\xi_{08,2})^8 = 0,37, \quad a_{8,3}(\xi_{08,3})^8 = 1,08.$$

We see that only the first solution

$$\begin{aligned} f(\xi) \quad = \quad & 1 - 0,44375\xi - 0,098456\xi^2 - 0,006711\xi^3 \\ & +3,801 \cdot 10^{-4}\xi^4 + 1,127 \cdot 10^{-5}\xi^{-5} - 5,430 \cdot 10^{-7}\xi^{-6} \\ & +5,799 \cdot 10^{-7}\xi^7 + 1,698 \cdot 10^{-8}\xi^8, \\ & \xi \le \xi_{08,1}, \quad \xi_{08,1} = 1,6161, \quad x_{08,1} = 1,6161\sqrt{D_s t} \end{aligned} \tag{2.14}$$

is defined with very high accuracy $a_8(\xi_{08,1})^8 = 7,9 \cdot 10^{-7}$ in the region $0 \le \xi \le \xi_{08,1}$. Including the above presented symmetry we have seven solutions. Two last solutions presented in Table 1 [4] do not satisfy the boundary condition $f(\xi_0) = 0$. Increasing the number of equations we can obtain more solutions. We chose the physical solution (2.14) comparing the maximum penetration with mean-square displacement $\sqrt{2D_s t}$ for the Braunian movement.

3. THE EXPANSION AT THE MAXIMUM PENETRATION POINT

The more successful solution of the nonlinear equation (1.1) can be obtained by expanding at the maximum penetration point of impurities. In this case the solution of the nonlinear equation (2.7) can be expressed in the following form

$$f(\xi) = \sum_{n=1}^{\infty} b_n(\xi - \xi_0)^n, \quad 0 \le \xi \le \xi_0. \tag{3.1}$$

Substituting the last expression in the modified equation (2.7)

$$2\frac{d}{d\xi}\left(f\frac{d}{d\xi}f\right) + (\xi - \xi_0)\frac{d}{d\xi}f + \xi_0\frac{d}{d\xi}f = 0. \tag{3.2}$$

we get the following relations between coefficients b_n

$$2n\sum_{m=1}^{n}(n+1-m)b_{n+1-m}b_m + (n-1)b_{n-1} + n\xi_0 b_n = 0. \tag{3.3}$$

From the last expression we can easy get the recurrent relations

$$b_1 = -\frac{1}{2}\xi_0, \quad b_n = \frac{2}{\xi_0}\left[\sum_{m=2}^{n-1}\frac{n+1-m}{n}b_{n+1-m}b_m + \frac{n-1}{2n^2}\cdot b_{n-1}\right]. \tag{3.4}$$

From the boundary conditions (2.9) and (3.1), (3.4) we obtain the equation for definition of maximum penetration point ξ_0

$$\sum_{n=1}^{\infty}(-1)^n(\xi_0)^n b_n - 1 = 0, \quad \xi_{0,n} = \left(\sum_{m=1}^{n}(-1)^m C_m\right)^{-\frac{1}{2}}, \quad C_m = b_m(\xi_0)^{m-2}. \tag{3.5}$$

Restricting expansion (3.1) by the six members and using (3.3) and (3.4) we obtain the following system of equations

$$\begin{aligned} 2b_1 + \xi_0 &= 0, \\ 12b_1b_2 + b_1 + 2\xi_0 b_2 &= 0, \\ 24b_1b_3 + 12(b_2)^2 + 2b_2 + 3\xi_0 b_3 &= 0, \\ 40b_2b_3 + 40b_1b_4 + 3b_3 + 4\xi_0 b_4 &= 0, \\ 60b_1b_5 + 60b_2b_4 + 30(b_3)^2 + 4b_4 + 5\xi_0 b_5 &= 0, \\ 84b_1b_6 + 84b_2b_5 + 84b_3b_4 + 5b_5 + 6\xi_0 b_6 &= 0, \\ -\xi_0 b_1 + (\xi_0)^2 b_2 - (\xi_0)^3 b_3 + (\xi_0)^4 b_4 - (\xi_0)^5 b_5 + (\xi_0)^6 b_6 - (\xi_0)^7 b_7 &= 1. \end{aligned} \tag{3.6}$$

This system of seven equations has six unknown coefficients b_i and ξ_0. The first six equations can be easily solved step by step beginning from the first. The accuracy of finding $\xi_{0,n}$ from the last equation depends on the number n of the equations and terms in expansion (3.1) We obtained the following exact results

$$\begin{aligned} &b_1 = -\frac{1}{2}\xi_0, b_2 = -\frac{1}{8}, b_3 = -\frac{1}{144\xi_0}, \\ &b_4 = -\frac{1}{1152(\xi_0)^2}, b_5 = -\frac{11}{172800(\xi_0)^3}, b_6 = -\frac{1}{230400(\xi_0)^4}, \end{aligned} \tag{3.7}$$

$$\begin{aligned} &\xi_{0,1} = \sqrt{2}, \quad \xi_{0,2} = \sqrt{\frac{8}{3}}, \quad \xi_{0,3} = \frac{12}{\sqrt{55}}, \quad \xi_{0,4} = \frac{24\sqrt{2}}{21}, \\ &\xi_{0,5} = \frac{120\sqrt{12}}{66161}, \quad \xi_{06} = \frac{10\sqrt{6912}}{\sqrt{264641}}. \end{aligned} \tag{3.8}$$

Using (3.4) and (3.5) we can get the infinite set of coefficients for infinite series (3.1) and ξ_0. In this case the analytical solution (3.1) can be obtained with desirable accuracy. We can get another set of the approximate solutions by taking the negative meanings of $\xi_{0,i}$ and by multiplying all coefficients b_n on $(-1)^n$. These solutions represent diffusion in the opposite direction of x axis. If b_n in (2.11) we replace by $c_n = \frac{1}{(\xi_0)^{n-2}}$ the obtained series converge for $0 < \xi \leq \xi_0$ according the D'Alembert's rule when $\xi_0 > 1$. Because (3.7) $b_i < c_i$ and $f(0) = 1$ series (3.1) also converge in the region $0 \leq \xi \leq \xi_0$.

The obtained results we can present in the form of theorem.

Theorem 3.1. *The asymptotical solution of nonlinear equation* (2.7) *is defined at the maximum penetration point* ξ_0.

We obtained that asimptotical solution of equation (2.7) with conditions (2.9) exist in the point ξ_0, $f(\xi_0) = 0$ and has main asymptotical term is $-\frac{1}{2}\xi_0(\xi - \xi_0)$ abound point ξ_0.

4. CONCLUSIONS

The more illustrative expressions of the similarity variables on the frontier of diffusion (3.7) can be presented approximately

$$\xi_{0,1} = 1,4142,\ \xi_{0,2} = 1,6330,\ \xi_{0,4} = 1,6162,\ \xi_{0,5} = 1,61611,\ \xi_{0,6} = 1,61612. \quad (4.1)$$

From these results, Table 1 [4] and (2.14) we see that $\xi_{0,5} = \xi_{08,1}$. $\xi_{08,1}$ – is obtained for physical solution (2.8) where terms till $a_8\xi^8$ are included. We can conclude that physical solutions coincide and converge independently on the different manners (2.8), (3.1) of expansion. Using the expansion (3.1), we got unique physical solution (3.4), (3.5). The maximum values (3.8) of the similarity variable in expansion (3.1) tend to the constant value faster than in the expansion about zero (2.8). The physical solution for the expansion (2.8) tend to exact solution faster than nonphysical solutions presented in Table 1. It gives the same depth of the impurities penetration like in expansion (3.1) where we got the unique solution. When we restrict the expansion (3.1) by five terms we get then from (3.7), (3.8)

$$f(\xi) = 1 - 0,44382\xi - 0,09832\xi^2 - 6,839\cdot 10^{-3}\xi^3 + 4,542\cdot 10^{-4}\xi^4 - 1,508\cdot 10^{-5}\xi^5,$$

$$0 \le \xi \le \xi_0, \quad \xi_0 = 1,6161. \quad (4.2)$$

After comparing the presented solution with the expansion at zero in [1] we found out that the obtained solutions practically coincide in the region $0 \le \xi \le \xi_0$. The problem of uniqueness of the solutions (2.8) of the diffusion equation (1.1) can not be solved including only one from the two boundary conditions (2.9). We obtained the unique analytical solution (3.1), (3.4), (3.5) including two boundary (2.9) conditions in one parametrical case.

From solutions (2.8), (2.10) which take into account only one boundary condition the correct physical solution can be separated from others by comparing the theoretical maximum penetration depths of the impurities with $\sqrt{2Dt}$.

The presented expansion (3.1) can be used successfully in the expression of the solutions for nonisothermical diffusion [6], [7].

REFERENCES

[1] A.J. Janavičius. Method for solving the nonlinear diffusion equation. *Physics Letters*, **A 224** , 1997, 159 – 162.

[2] Simone Artz, Michael Schulz, Steffen Trimper. Diffusion with restrictions. *Physics Letters*, **A 244** , 1998, 172 – 276.

[3] B.F. Apostol. On a non-linear diffusion equation deseveling clouds and wreaths of smoke. *Physics Letters*, **A 235** , 1997, 363 – 366.

[4] A.J. Janavičius, P. Norgėla. Problem of uniqueness of the physical solution of nonlinear diffusion equation. *ŠU Fizikos ir matematikos fakulteto seminaro darbai*, **1** , 1998, 5 – 9.

[5] C. Kittel. *Elementary statistical physics*. Wiley, New York, 278, 1958.

[6] A.J. Janavičius. The nonlinear diffusion in the nonisotermical case. *Acta Physica Polonica*, **A 93** , 1998, 505 – 512.

[7] A.J. Janavičius. Nonlinear diffusion in exited systems. *Lithuanian Journal of Physics*, **37** (6), 1997, 508.

NETIESINĖS DIFUZIJOS LYGTIES ANALIZINIO SPRENDINIO VIENATINUMAS IR KONVERGAVIMAS

A.J. JANAVIČIUS, P. NORGĖLA, D. JURGAITIS

Klasikinė tiesinė difuzijos lygtis yra išvesta iš Fokerio-Planko lygties darant prielaidą, kad difuzijos procesas yra lėtas. Tačiau tai negali būti taikoma klasikinės tiesinės difuzijos lygties sprendinio $erfc(x/2\sqrt{Dt})$ asimptotikai, aprašančiai difunduojančių priemaišų įsiskverbimą medž]iagoje neribotai dideliuose atstumuose x. Iš Brauno judėjimo teorijos seka, kad per baigtinį laiką t difunduojančios dalelės gali įsiskverbti medž]iagoje tik iki baigtinio atstumo nuo difunduojančių dalelių šaltinio, kuris apytikriai lygus vidutiniam kvadratiniam difunduojančių dalelių poslinkiui $\sqrt{2Dt}$). Netiesinė difuzijos lygtis pakankamai tiksliai aprašanti difunduojančių priemaišų pasiskirstymą puslaidininkiuose gauta padarius prielaidą, kad difunduojančių dalelių srauto tankis yra apibrėžiamas difuzijos koeficientu D proporcingu priemaišų koncentracijai N. Tuomet srityje, kur priemaišų koncentracija lygi nuliui, difuzijos koeficientas lygus nuliui taip pat. Taip užtikrinama fizikinė sąlyga, kad per baigtinį laiką priemaišos medžiagoje turi įsiskverbti į baigtinį gylį.

Darbe išdėstytas netiesinės difuzijos lygties sprendimas, nagrinėjant vienmatę difuziją iš begalinio šaltinio (kai kieto kūno paviršiuje priemaišų koncentracija N_S yra pastovi), laipsninėmis eilutėmis dviem skirtingais būdais.