International Journal of Modern Mathematical Sciences, 2024, 22(1): 15-24

International Journal of Modern Mathematical Sciences ISSN:2166-286X

Journal homepage:www.ModernScientificPress.com/Journals/ijmms.aspx Florida, USA

Article

Application of Akbari – Ganji's Method in Solving a Surface Coverage Model

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Article history: Received 15 March 2024, Revised 4 June 2024, Accepted 7 June 2024, Published 11 June 2024.

Abstract: A surface coverage model in an electrochemical arsenic sensor is solved analytically using Akbari-Ganji's method. It is found that the solution derived using this method makes a very good fit with the numerical simulation. This method seems to be very efficient in obtaining the closest solution to the nonlinear model. The analytical solution obtained will help in predicting the relationship between the parameters and the model results.

Keywords: Reaction-diffusion equations, Surface coverage model, Michaelis – Menten constant, Akbari– Ganji's method, Numerical simulation

Mathematics Subject Classification: 34E, 35K20 and 68U20

1. Introduction

The World Health Organization states that arsenic is a naturally occurring substance found in the earth's crust and is extensively dispersed across the air, water, and land. In its inorganic form, it is extremely poisonous. Eating contaminated food, smoking tobacco, using polluted water in industrial processes, drinking contaminated water for food preparation and crop irrigation, and eating contaminated food can all expose people to high doses of inorganic arsenic. Chronic arsenic poisoning can result from long-term exposure to inorganic arsenic, mostly from food and drinking water. The most common side effects include skin blemishes and skin cancer. The source of the biggest arsenic threat to public health is tainted groundwater. Many nations' ground waters, including those in Argentina, Bangladesh, Chile, China, India, Mexico, and the United States of America, naturally have high concentrations of inorganic arsenic. The sources of exposure are polluted drinking water, irrigated crops, and food prepared with contaminated water.

Sensors are analytical devices utilized for the recognition of chemical substances in a solution to be analyzed. Widespread use of computational modeling is made to enhance sensor design and optimize settings. An electrochemical sensor's surface coverage parameter is essential for improving the sensor's figure of merit. The production of functional electrodes for electrochemical sensors can be standardized with the aid of a theoretical model for surface coverage. A surface coverage model for an electrochemical arsenic sensor was presented by Sathiyaseelan et al. [1]. This model was mathematically studied by Ananthaswamy et al. [2] using the new homotopy perturbation method. The goal of this work is to solve this nonlinear model by applying the Akbari-Ganji approach.

2. Mathematical Formulation of the Problem

Sathiyaseelan et al.[1] developed the differential mass balance for arsenic in the case of arsenic-F-doped CdO catalytic reaction, in an unsteady state as follows

$$\frac{\partial[As]}{\partial t} = D_{[As]}\frac{\partial^2[As]}{\partial x^2} - \frac{I_{\max}[As]}{K_M + [As]} \tag{1}$$

where $[As]$ is the arsenic concentration, $D_{[As]}$ is the diffusion coefficient of arsenic, t is time, x is the thickness of the F-doped CdO thin film electrode, $I_{\max}$ is the maximum current response and K_M is the Michaelis Menten constant. In their work, the diffusion layer was defined as the region in the vicinity of F-doped CdO thin film electrode where the concentration of arsenic is different from its value in the bulk solution (0.4 M NaCl).

The initial and boundary conditions are as follows

$$x = 0,\ \frac{\partial[As]}{\partial x} = 0 \tag{2}$$

$$x = d,\ [As] = As_0 \tag{3}$$

$$t = 0,\ [As] = 0 \tag{4}$$

Ananthaswamyet al.[2] introduced the following dimensionless variables to convert the model to the dimensionless form

$$A = \frac{[As]}{As_0},\ X = \frac{x}{d},\ \tau = \frac{D_{[As]}t}{d^2} \tag{5}$$

The dimensionless form of the model is

$$\frac{\partial A}{\partial \tau} = \frac{\partial^2 A}{\partial X^2} - \phi^2\left(\frac{A}{\alpha + A}\right) \tag{6}$$

$$X = 0,\ \frac{\partial A}{\partial X} = 0 \tag{7}$$

$$X = 1,\ A = 1 \tag{8}$$

$$\tau = 0,\ A = 0 \tag{9}$$

The steady state of the above model is

$$\frac{d^2 A}{dX^2} - \phi^2\left(\frac{A}{\alpha + A}\right) = 0 \tag{10}$$

$$X = 0,\ \frac{dA}{dX} = 0 \tag{11}$$

$$X = 1,\ A = 1 \tag{12}$$

3. Analytical Solution to Eqns. (10) to (12) Using Akbari-Ganji's Method

Various analytical methods like homotopy perturbation method [3-19], homotopy analysis method [20-22], Adomian decomposition method [23], wavelet transform method, etc. are efficient methods to solve nonlinear differential equations. In this paper Akbari–Ganji's method [24, 25] is applied to find the analytical expression for the dimensionless arsenic concentration.

Consider an initial guess that satisfies eqns (11) and (12) as follows

$$A = \frac{\cosh(bX)}{\cosh(b)}, \tag{13}$$

where b is the constant coefficient

Substituting eqn (13) in eqn (10),

$$\frac{b^2}{\cosh b} - \phi^2\left[\frac{1}{\alpha \cosh b + \cosh bx}\right] = 0 \tag{14}$$

At $x = 1$, the above equation gives

$$b = \frac{\phi}{\sqrt{\alpha + 1}} \tag{15}$$

Hence the approximate analytical expression for the dimensionless arsenic concentration is

$$A = \frac{\cosh\left(\frac{\phi}{\sqrt{\alpha+1}} X\right)}{\cosh\left(\frac{\phi}{\sqrt{\alpha+1}}\right)}$$

4. Numerical Simulation

Numerical solutions are also obtained for the non-linear differential equations (10) through (12). The problem has been numerically solved using MATLAB software and the pdex4 function. A comparison is made between the numerical simulation and the acquired analytical results. The MATLAB program is given in Appendix C.

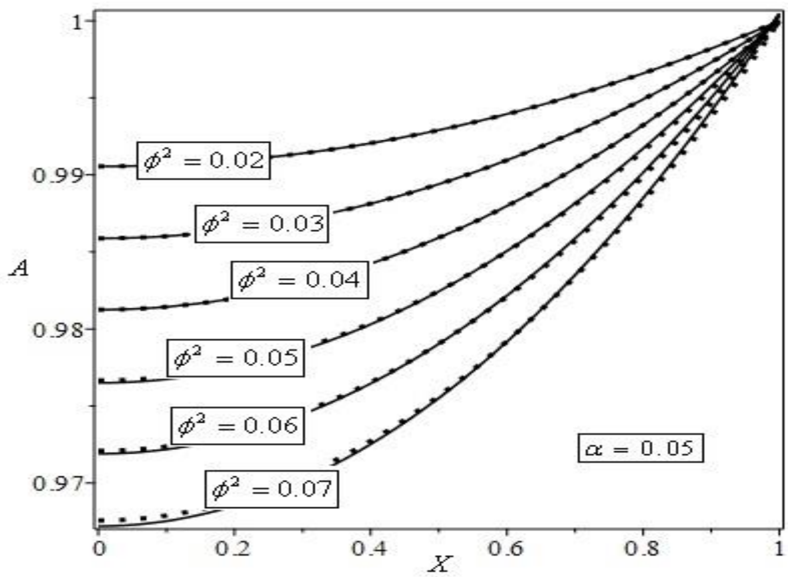

Figure 1. Plot of dimensionless concentration of arsenic(A) versus dimensionless thickness of the F-doped CdO electrode(X) for various values of ϕ^2. The dotted lines represent the analytical solution and solid lines represent the numerical simulation.

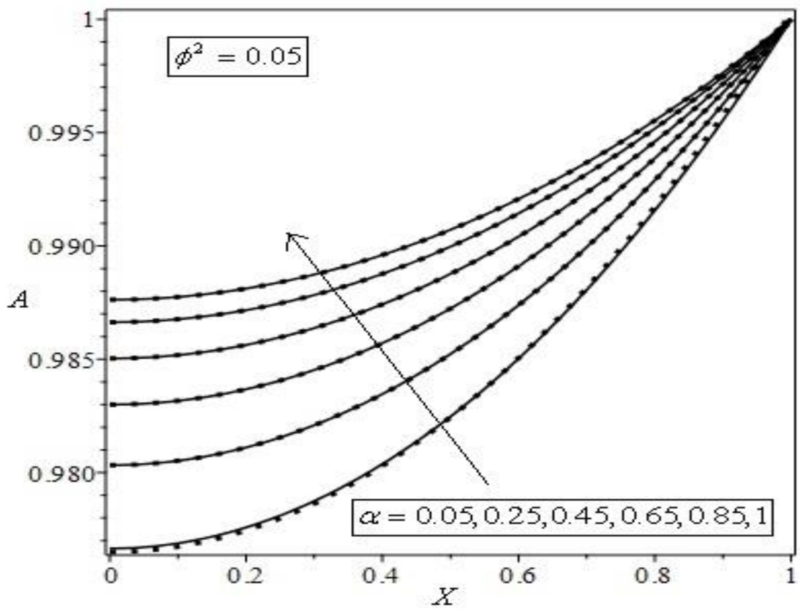

Figure 2. Plot of dimensionless concentration of arsenic(A) versus dimensionless thickness of the F-doped CdO electrode(X) for some fixed values of parameters and various values of α. The dotted lines represent the analytical solution and solid lines represent the numerical simulation.

5. Results and Discussion

The Akbari–Ganji approach has been used to generate the analytical expression for the dimensionless arsenic concentration. When the generated analytical solution and the numerical simulation are compared, they are found to fit quite well. Further examination of figures 1 and 2 reveals that ϕ^2 has a negative influence on the dimensionless arsenic concentration while α has a favorable impact on it. Appendix A provides an overview of the Akbari-Ganji approach.

6. Conclusion

In this paper, a surface coverage model pertaining to an electrochemical arsenic sensor is solved analytically using Akbari– Ganji's method to obtain an approximate analytical expression for the dimensionless arsenic concentration. The obtained analytical results will aid in the researchers' interpretation of the impact of various parameters on the concentration of arsenic in water. In addition, the Akbari–Ganji approach seems to be a simple and effective way to solve mathematical models that are nonlinear.

Appendix A

Basic Concept of Akbari-Ganji's Method

Consider the following nonlinear differential equation and boundary conditions

$$f\left(u'', u', u, F_o(\sin\omega t)\right) = 0 \tag{A.1}$$

$$u(0) = A, \quad u'(0) = B \tag{A.2}$$

Choose an initial guess which satisfies eqn. (A.2), as follows

$$u(x) = e^{-at}\{b\cos(\omega t + \phi)\} \tag{A.3}$$

where $\{a, b, \omega, \phi\}$ are constant coefficients

Using the initial conditions of eqn.(A.2) the following two cases arises

$$(a) \qquad u(t) = u(IC) \tag{A.4}$$

$$(b) \qquad u(t) = g(t) \tag{A.5}$$

Substituting eqn.(A.5) in eqn.(A.1), we get

$$f(t) = f\left(g''(t), g'(t), g(t), F_o(\sin\omega t)\right) = 0 \tag{A.6}$$

Substituting eqn.(A.4) in eqn. (A.6) and its derivatives, the following is obtained

$$f(IC) = f\left(g''(IC), g'(IC), g(IC), ...\right) = 0 \tag{A.7}$$

$$f'(IC) = f\left(g''(IC), g'(IC), g(IC), ...\right) = 0 \tag{A.8}$$

$$f''(IC) = f\left(g''(IC), g'(IC), g(IC), ...\right) = 0 \tag{A.9}$$

From eqn.(A.7), the set of n-algebraic equations with n-unknowns can be determined.

From these equations, the constant coefficients $\{a, b, \omega, \phi\}$ can be obtained.

Appendix: B

Nomenclature

Symbols	Meaning
$[As]$	arsenic concentration in μM
$D_{[As]}$	diffusion coefficient of arsenic in cm^2/s
$I_{\max}$	maximum current response in μA
K_M	Michaelis – Menten constant in μM
x	thickness of the F-doped CdO thin film electrode in cm
t	time in s
ϕ^2	Thiele modulus
α	saturation parameter

A	dimensionless arsenic concentration
X	dimensionless thickness of the F-doped CdO thin film electrode
τ	dimensionless time

Appendix: C

MATLAB program to find the numerical solution of eqns. (10)-(12)

```
function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,1000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,2)')
%------------------------------------------------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1];
f = [1] .* DuDx;
p=0.9;
a=0.5;
F=-((p*u(1))/(a+u(1)));
s=[F];
% ---------------------------------------------
function u0 = pdex4ic(x);
u0 = [0];
% ---------------------------------------------
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = [0];
ql = [1];
pr = [ur(1)-1];
qr = [0];
```

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