ijndes
Published by Global Research Publications, New Delhi, India

OZONE DECOMPOSITION OF THE SECOND ORDER IN AQUEOUS SOLUTION BY VARIATIONAL ITERATION METHOD

J. Biazar [a,*], M. Shahbala[a] & H. Ebrahimi[b]

[a]*Department of Mathematics, Faculty of Science, University of Guilan, P.O.Box.41635-19141, P.C. 4193833697, Rasht, Iran.*

[b]*Department of Mathematics, Islamic Azad University (branch:Rasht), P. O. Box 41335-3516, Rasht, Iran.*

Received: 11th April 2016, Accepted: 12th June 2016

Abstract: *In this paper the problem of mass transfer of ozone of the second order from a gaseous phase into an aqueous phase has been studied. And He's variational iteration method is applied to derive an analytical approximation to the solutions of the system of differential equations governing on the problem. Some parametric studies have also been included. To illustrate the effects of the temperature and hydroxyl ion reaction order to the solutions, some plots are provided.*

Keywords: *He's Variational Iteration Method; Ozone Decomposition.*

1. INTRODUCTION

The use of ozone has been shown to be efficient in activating pathogens and reducing bacterial gill disease in freshwater re-circulation systems. Even in marine systems, for handling environmental contaminants, the use of ozone, is increasingly becoming very popular. Furthermore, ozone has been shown to improve water quality by oxidizing nitrite, natural organic matter (NOM), ammonia, and removal of fine suspended particles as well as re-oxygenation of the water [1,2].

The ozone demand and decomposition behavior in aqueous solutions need to be quantified. In this study, the ozone decomposition kinetics is being investigated. Applying He's variational iteration method, for the first time, solves non-linear equations, governing the problem. This reliable analytic approximation to the solution is of great interest. The main reason of this interest is that this analytic approximation can be used in many engineering purposes, using this analytic approximation one can easily study the effects of different parameters to the solution. Mathematical modeling of the problem leads to the following system of two non-linear differential equations:

[*] Corresponding Author: *Jafar.biazar@gmail.com, ebrahimi.hamideh@gmail.com*

$$\begin{cases} \dfrac{dC(t)}{dt} = -K_D C(t)^2 - K_R D(t)C(t), \\ \dfrac{dD(t)}{dt} = -K_R D(t)C(t). \end{cases} \tag{1}$$

Where $D(t)$ concentration of NOM fraction with fast ozone demand (mg/l); $C(t)$ dissolved oxygen concentration at time t (mg/l); K_R first-order ozone decomposition rate constant (1/min); and K_R second-order rate constant (1/mg min).

Biazar, Tango and Islam [3] used Adomian decomposition method (ADM) to solve this problem. A substantial amount of numerical and analytical work has been done on this work.

2. HE'S VARIATIONAL ITERATION METHOD

This method, which has been developed by J. He, (1998), [4-6], is a popular device for solving various non-linear equations.[7-8] To illustrate the basic idea of the method, consider the following general non-linear system:

$$Lu(t) + Nu(t) = g(t). \tag{2}$$

Where L is a linear operator, N is a nonlinear operator, and $g(t)$ is a known analytical function. According to variational iteration method, we can construct the following correction functional:

$$u_{n+1}(t) = u_n(t) + \int_0^t \lambda(\xi)(Lu_n(\xi) + N\tilde{u}_n(\xi) - g(\xi))d\xi. \tag{3}$$

Where λ is a general Lagrange multiplier [9], that can be identified optimally via variational theory [10-11], $\tilde{u}_n$ is considered as restricted variation [11], i.e., $\delta\tilde{u}_n = 0$, and $u_0(t)$ is an initial approximation with possible unknowns. For linear problems, exact solution can be obtained by only one iteration, because λ can be identified exactly.

3. SOLUTION OF SYSTEM (1) BY VARIATIONAL ITERATION METHOD

For solving system (1), correction functional can be written down as follows:

$$\begin{cases} C_{n+1}(t) = C_n(t) + \int_0^t \lambda_1(\xi)\left(\dfrac{dC_n}{d\xi} + K_D\tilde{C}_n(\xi)^2 + K_R\tilde{C}_n(\xi)\tilde{D}_n(\xi)\right)d\xi, \\ D_{n+1}(t) = D_n(t) + \int_0^t \lambda_2(\xi)\left(\dfrac{dD_n}{d\xi} + K_R\tilde{C}_n(\xi)\tilde{D}_n(\xi)\right)d\xi. \end{cases} \tag{4}$$

Making the above correct functional stationary and considering noticing that $\delta C_n(0) = 0, \delta D_n(0) = 0,$

we have,

$$\begin{cases} \delta C_{n+1}(t) = \delta C_n(t) + \lambda_1(\xi)\delta C_n(\xi)\Big|_0^t - \int_0^t \dfrac{d\lambda_1}{d\xi}\delta C_n(\xi)d\xi = 0, \\ \delta D_{n+1}(t) = \delta D_n(t) + \lambda_2(\xi)\delta D_n(\xi)\Big|_0^t - \int_0^t \dfrac{d\lambda_2}{d\xi}\delta D_n(\xi)d\xi = 0. \end{cases}$$

The stationary conditions can be obtained as follows:

$$\begin{cases} \delta C_n: \begin{cases} 1+\lambda_1(t)=0, \\ \dfrac{d\lambda_1(\xi)}{d\xi}=0, \end{cases} \\ \delta D_n: \begin{cases} 1+\lambda_2(t)=0, \\ \dfrac{d\lambda_2(\xi)}{d\xi}=0. \end{cases} \end{cases} \tag{5}$$

From this, the Lagrange multipliers can be identified as $\lambda_1=\lambda_2=-1$, so we obtain the following iteration formula:

$$\begin{cases} C_{n+1}(t)=C_n(t)-\int_0^t \left(\dfrac{dC_n}{d\xi}+K_D C_n(\xi)^2+K_R C_n(\xi)D_n(\xi)\right)d\xi, \\ D_{n+1}(t)=D_n(t)-\int_0^t \left(\dfrac{dD_n}{d\xi}+K_R C_n(\xi)D_n(\xi)\right)d\xi. \end{cases} \tag{6}$$

Beginning with $C_0 = C(0)$, $D_0 = D(0)$, by iteration formula (6) we have,

$$\begin{aligned} C_1 &= \left(-k_2C_0^2-k_1C_0D_0\right)t+C_0, \\ D_1 &= -k_1C_0D_0t+D_0, \\ C_2 &= \left(-\frac{1}{3}k_2\left(-k_2C_0^2-k_1C_0D_0\right)^2+\frac{1}{3}k_1^2\left(-k_2C_0^2-k_1C_0D_0\right)C_0D_0\right)t^3+ \\ &\quad \left(-k_2C_0\left(-k_2C_0^2-k_1C_0D_0\right)+\frac{1}{2}k_1^2C_0^2D_0-\frac{1}{2}k_2\left(-k_2C_0^2-k_1C_0D_0\right)D_0\right)t^2 \\ &\quad +\left(-k_2C_0^2-k_1C_0D_0\right)t+C_0, \\ D_2 &= \frac{1}{3}k_1^2\left(-k_2C_0^2-k_1C_0D_0\right)C_0D_0t^3+\left(\frac{1}{2}k_1^2C_0^2D_0-\frac{1}{2}k_1\left(-k_2C_0^2-k_1C_0D_0\right)\right. \\ &\quad \left.D_0\right)t^2-k_1C_0D_0t+D_0, \\ &\quad \vdots \end{aligned}$$

4. NUMERICAL STUDY AND DISCUSSION

For numerical study let us start with stating the relationship of K_D and K_R with other parameters as:

$$\begin{aligned} K_D &= A_D\left[OH^-\right]^x \exp\left(-\frac{E}{RT}\right), \\ K_R &= A_R\left[OH^-\right]^x \exp\left(-\frac{E}{RT}\right). \end{aligned} \tag{7}$$

Where A_D and A_R are frequency factors for ozone decomposition reactions (1/min); [OH^-] is concentration of hydroxide ion (mol/l); X reaction order; E activation energy (kcal/mol); R is gas constant (kJ/K mol) and T is temperature (K).

Table 1
The Model Parameters and Constants

Parameter	*Values*
E, kcal/ mol	8.0×10^4
R, kJ/K mol	8.314
A_D, 1/min	10^9
A_R, 1/min	0.5×10^9
C (0), mg/l	2
D (0), mg/l	10^{-5}
OH	3.12764

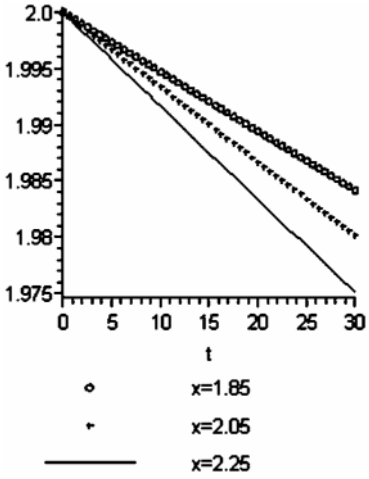

Figure. 1: Plots of the Second-order Reaction for different Values of x Versus Time.

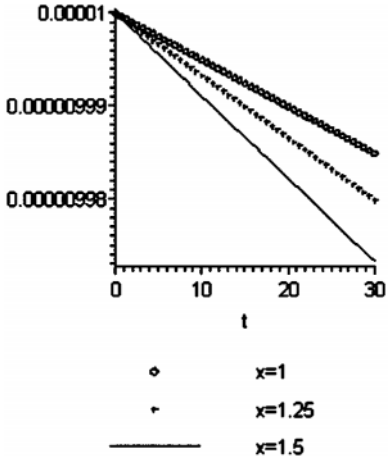

Figure. 2: Plots of the Second-order Reaction NOM for different Values of x Versus Time.

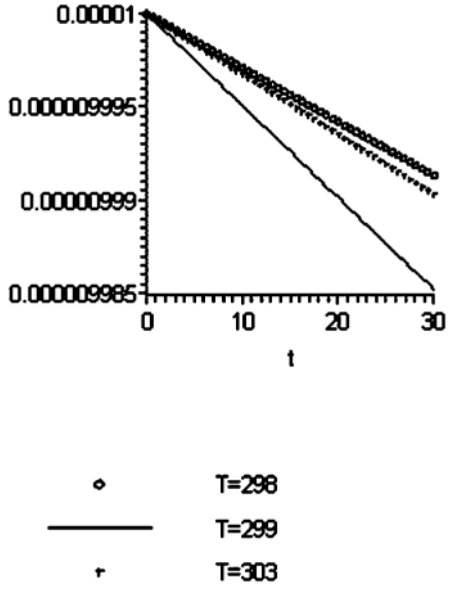

Figure. 3: Plots of the Second-order Reaction NOM for different Temperatures Versus Time.

In this study the values of Table 1 are considered.

Fig. 1 shows the effect of hydroxyl ion reaction order on the ozone decomposition. Ozone decomposes at a faster rate as the reaction order of the hydroxyl ion increases.

Fig. 2 shows the effect of hydroxyl ion reaction order on the degradation of the natural organic matter. The NOM degrades at a faster rate as the reaction order of the hydroxyl ion increases.

Fig. 3 shows the effect of temperature on the degradation of the natural organic matter. The NOM degrades at a faster rate as the temperature increases.

REFERENCES

[1] S. T. Summer Felt, J.A. Hankins, A.L. Weber, M. D. Durant, "Ozonation of a Re-circulating Rainbow Trout Culture System. II", *Effects on Micro Screen Filtration and Water Quality*, *Aquaculture*, **158,** 1997, 57-67.

[2] G.L. Lucchetti, G.A. Gray, "Water Reuses Systems, a Review of Principal Components", *Prog. Fish Culturist*. **50,** 1988, 1-6.

[3] J. Biazar, M. Tango, R. Islam, "Ozone Decomposition of the Second Order in Aqueous Solutions", *Applied Mathematics and Computation*, **177,** 2006, 220-225.

[4] J. H. He, "Variational Iteration Method-a kind of Non-linear Analytical Technique: Some Examples", *International Journal of Nonlinear Mechanics*, **34 (4),** 1999, 699-708.

[5] J. H. He, "Some Asymptotic Methods for Strongly Nonlinear Equations", *International Journal of Modern Physics*, B **20** (10), 2006, 1141-1199.

[6] J. H. He, "Non-perturbative Methods for Strongly Nonlinear Problems", *Dissertation, de-Verlag in Internet GmbH*, Berlin, 2006.

[7] Biazar, H. Ghazvini, "He's Variational Iteration Method for Solving Hyperbolic Differential Equations", *International Journal of Nonlinear Sciences and Numerical Simulation*, **8(3)**, 311-314, 2007.

[8] D. D. Ganji, M. Nourollahi, E. Mohseni, "Application of He's Methods to Nonlinear Chemistry Problems", *Computers and Mathematics with Applications*, **54 (7-8),** 2007, 1122-1132.

[9] M. Inokuti et al., "General use of the Lagrange Multiplier in Non-linear Mathematical Physics", in: S. Nemat-Nasser (Ed.), *Variational Method in the Mechanics of Solids*, Pergamon Press, Oxford, 1978, pp. 156-162.

[10] J. H. He, "Semi-inverse Method of Establishing Generalized Principles for Fluid Mechanics with Emphasis on Turbo Machinery Aerodynamics", *International Journal of Turbo Jet-Engines*, **14 (1)**, 1997, 23-28.

[11] B. A. Finlayson, "The Method of Weighted Residuals and Variational Principles", Academic Press, New York, 1972.