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Analytical Solution for the Mass Transfer of Ozone of the Second Order from Gaseous Phase to Aqueous Phase†

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In this work, we consider the problem of mass transfer of ozone of the second order from a gaseous phase into an aqueous phase by employing the homotopy perturbation method. The series solution of the governing system of differential equations is obtained. Some examples have been included. The effects of the temperature and hydroxyl ion reaction order to the solutions are illustrated by some plots.

Key Words: Homotopy perturbation method, Analytical solution, Mass transfer of ozone.

INTRODUCTION

In this paper, the ozone kinetics is being investigated by using the homotopy perturbation method. The use of ozone has been shown to be efficient in inactivating 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, ammonia and removal of fine suspended particles as well as re-oxygenation of the water[1,2]. Non-linear equations, governing to the problem, are solved by applying homotopy perturbation method for the first time. This reliable analytic approximation to the solution is of great interest. Mathematical modelling of the problem leads to the following system of two non-linear differential equations:

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

where D(t) is the concentration of neutral organic matter fraction with fast ozone demand (mg/L); C(t), dissolved oxygen concentration at time t (mg/L); K_D, first-order ozone decomposition rate constant (1/min); K_R, second-order rate constant (1/mg min). Recently, Biazar *et al.*[3] used Adomian decomposition method for solving the governing problem. In this study, we will use homotopy perturbation method to obtain analytical solution for the problem of mass transfer of ozone of the second order from a gaseous phase into an aqueous pahse.

The homotopy perturbation method was first proposed by Ji-Huan He[4-6]. The essential idea of this method is to introduce a homotopy parameter, say p, which takes values from 0 to 1. When p = 0, the system of equations usually reduces to a sufficiently simplified form, which normally admits a rather simple solution. As p is gradually increased to 1, the system goes through a sequence of deformations, the solution for each of which is close to that at the previous stage of deformation. Eventually at p = 1, the system takes the original form of the equation and the final stage of deformation gives the desired solution. One of the most remarkable features of the homotopy perturbation method is that usually just a few perturbation terms are sufficient for obtaining a reasonably accurate solution. This technique has been employed to solve a large variety of linear and non-linear problems[7-16]. This technique is further applied by He[17-20].

Solution by the homotopy perturbation method: In order to solve eqn. 1 by homotopy perturbation method, we construct the following homotopies:

$$\frac{dC(t)}{dt} = p\left[-K_D C^2(t) - K_R D(t)C(t)\right] \quad (2)$$

$$\frac{dD(t)}{dt} = p\left[-K_R D(t)C(t)\right] \quad (3)$$

Assume the solution of eqn. 1 in the forms:

$$C = C_0 + pC_1 + p^2C_2 + p^3C_3 + ... \quad (4)$$

$$D = D_0 + pD_1 + p^2D_2 + p^3D_3 + ... \quad (5)$$

†Dedicated to Prof. Dr. Azmi Telefoncu.

Substituting eqns. 4-5 into eqns. 2-3 and collecting terms of the same power of p, we get the following set of differential equations:

$$\begin{aligned}
&p^0 : \frac{dC_0(t)}{dt} = 0,\\
&p^1 : \frac{dC_1(t)}{dt} = -K_D(C_0(t)C_0(t)) - K_R(D_0(t)D_0(t)),\\
&p^2 : \frac{dC_2(t)}{dt} - K_D(2C_0(t)C_1(t)) - K_R(D_0(t)C_1(t) + D_1(t)C_0(t)),\\
&p^3 : \frac{dC_3(t)}{dt} - K_D(2C_0(t)C_2(t) + C_1^2(t)) - K_R(D_0(t)C_2(t) + D_1(t)C_1(t) + D_2(t)C_0(t)),\\
&\vdots
\end{aligned} \tag{6}$$

and

$$\begin{aligned}
&p^0 : \frac{dD_0(t)}{dt} = 0,\\
&p^1 : \frac{dD_1(t)}{dt} = -K_R(D_0(t)C_0(t)),\\
&p^2 : \frac{dD_2(t)}{dt} - K_R(D_0(t)C_1(t) + D_1(t)C_0(t)),\\
&p^3 : \frac{dD_3(t)}{dt} - K_R(D_0(t)C_2(t) + D_1(t)C_1(t) + D_2(t)C_0(t)),\\
&\vdots
\end{aligned} \tag{7}$$

Using eqns. 6 and 7, we obtain the following iterative formula:

$$C_0(t) = C(0), \tag{8}$$

$$D_0(t) = D(0), \tag{9}$$

$$C_j(t) = \int_0^t -(D_D A_j + K_R B_j)ds, \quad j \geq 0 \tag{10}$$

$$D_j(t) = \int_0^t -K_R(B_j)ds, \quad j \geq 0 \tag{11}$$

where

$$A_j = \sum_{i=0}^{j} C_i(s)C_{j-i}(s) \quad \text{and} \quad B_j = \sum_{i=0}^{j} D_i(s)C_{j-i}(s).$$

If we solve the above equation system 8-11, we successively obtain:

$$\begin{aligned}
&C_0(t) = C(0),\\
&C_1(t) = -C(0)(K_D C(0) + K_R D(0))t,\\
&C_2(t) = \frac{1}{2}C(0)(2C^2(0)K_D^2 + 3C(0)D(0)K_D K_R + D^2(0)K_R^2 + C(0)D(0)K_R^2)t^2,\\
&C_3(t) = \frac{1}{6}C(0)(6C^3(0)K_D^3 + 12C^2(0)D(0)K_D^2 K_R + 7C(0)D^2(0)K_D K_R^2 +\\
&\quad 5C^2(0)D(0)K_D K_R^2 + 5C^2(0)D(0)K_D K_R^2 + D^3(0)K_R^3 +\\
&\quad 4C(0)D^2(0)K_R^3 + C^2(0)D(0)K_R^3)t^3,\\
&\vdots
\end{aligned}$$

and

$$\begin{aligned}
&D_0(t) = D(0),\\
&D_1(t) = -K_R D(0)C(0)t,\\
&D_2(t) = \frac{1}{2}C(0)D(0)K_R(C(0)K_D + D(0)K_R + C(0)K_R)t^2,\\
&D_3(t) = \frac{1}{6}C(0)D(0)K_R(2C^2(0)K_D^2 + 3C(0)D(0)K_D K_R + D^2(0)K_R^2 +\\
&\quad 4C(0)D(0)K_R^2 + 3C^2(0)K_R K_D + C^2(0)K_R^2)t^3,\\
&\vdots
\end{aligned}$$

and so on; in this manner, the rest of the components of the homotopy perturbation series can be obtained. Then the series solutions expression by HPM can be written in the form:

$$\begin{aligned}
C(t) &= C_0(t) + C_1(t) + C_2(t) + C_3(t) + \ldots\\
D(t) &= D_0(t) + D_1(t) + D_2(t) + D_3(t) + \ldots
\end{aligned}$$

But for practical numerical computations, we shall use the finite 4-terms approximation of C(t) as $C(t) \approx \sum_{i=0}^{3} C_i$ and the 4-terms approximation of D(t) as $\approx \sum_{i=0}^{3} D_i$.

These approximations are presented as follows:

$$\begin{aligned}
&C(t) \approx C(0) - (K_D C^2(0) + K_R C(0)D(0))t +\\
&\left(C^3(0)K_D^2 + \frac{3}{2}C^2(0)D(0)K_D K_R + \frac{1}{2}C(0)D^2(0)K_R^2 + \frac{1}{2}C^2(0)D(0)K_R^2\right)t^2\\
&-\left(C^4(0)K_D^3 + 2C^3(0)D(0)K_D^2 K_R + \frac{7}{6}C^2(0)D^2(0)K_D K_R^2 +\right.\\
&\frac{5}{6}C^3(0)D(0)K_D K_R^2 + \frac{1}{6}C(0)D^3(0)K_R^3 + \frac{1}{6}C(0)D^3(0)K_R^3 +\\
&\left.\frac{2}{3}C^2(0)D^2(0)K_R^3 + \frac{1}{6}C^3(0)D(0)K_R^3\right)t^3,
\end{aligned}$$

and

$$\begin{aligned}
&D(t) = D(0) - (K_R D(0)C(0))t + \left(\frac{1}{2}C^2(0)D(0)K_D K_R + \frac{1}{2}C(0)D^2(0)K_R^2 +\right.\\
&\left.\frac{1}{2}C^2(0)D(0)K_R^2\right)t^2 - \left(\frac{1}{3}C^3(0)D(0)K_D^2 K_R + \frac{1}{2}C^2(0)D^2(0)K_D K_R^2 +\right.\\
&\frac{1}{6}C(0)D^3(0)K_R^3 + \frac{2}{3}C^2(0)D^2(0)K_R^2 + \frac{1}{2}C^3(0)D(0)K_D K_R^2 +\\
&\left.\frac{1}{6}C^3(0)D(0)K_R^3\right)t^3.
\end{aligned}$$

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

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

where A_D and A_R, frequency factors for ozone decomposition reactions (1/min); $[OH^-]$, concentration of hydroxide ion (mol/l); x , reaction order ; E, activation energy (kcal/mol); R, gas constant (kJ/K mol); T, temperature (K). In this study the values in Table-1 considered.

Fig. 1 presents the behaviour of ozone concentration and natural organic matter, the values of the parameters from Table-1 are substituted in the solutions and Fig. 1 shows the changes in residual ozone with time. The results suggest that ozone decomposes at a faster rate as with increases in the reaction order of the hydroxyl ion.

TABLE-1
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^-	0.8×10^9

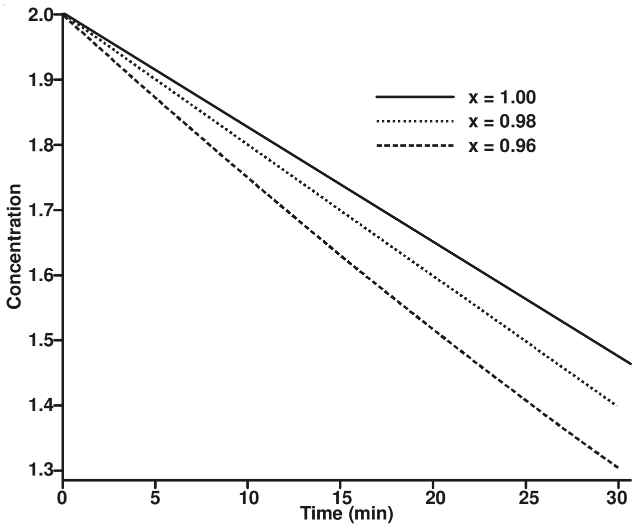

Fig. 1. Plots of the second-order reaction for different values of x *versus* time

Fig. 2 shows the effect of temperature on the ozone decomposition. The residual ozone concentration decreases at a faster rate, as temperature of the marine water was increase from 5 to 15 ºC.

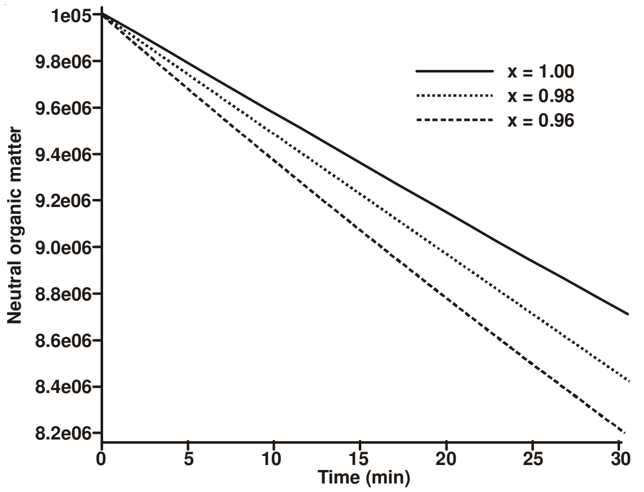

Fig. 2. Plots of the second-order reaction neutral organic matter for different values of x *versus* time

Fig. 3 shows the effect of hydroxyl ion reaction order on the degradation of the natural organic matter. The neutral organic matter degrades at a faster rate as the reaction order of the hydroxyl ion decreases.

Fig. 4 shows the effect of temperature on the degradation of the natural organic matter. The neutral organic matter degrades at a faster rate as the temperature increases.

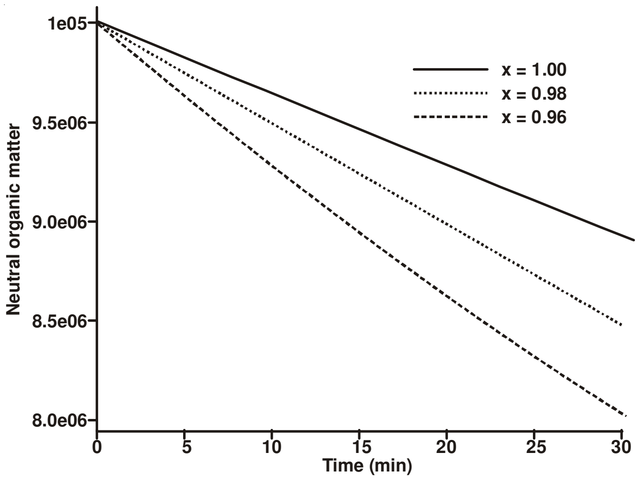

Fig. 3. Plots of first-order reaction neutral organic matter *versus* time

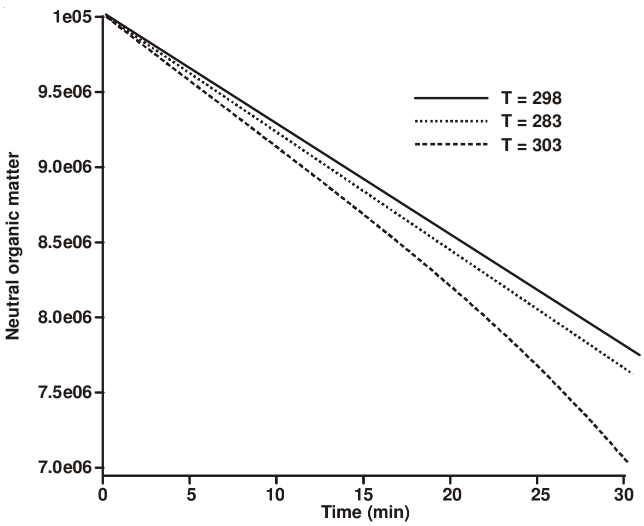

Fig. 4. Plots of the second-order reaction neutral organic matter for different temperatures *versus* time

Conclusion

In this paper, the homotopy perturbation method was employed to solve the problem of mass transfer of ozone of the second order in aqueous. We obtained the approximate analytical solution of the equation in the form of a convergent power series with easily computable components. The method needs much less computational work compared with traditional methods. The method is extremely simple, easy to use and is accurate for solving nonlinear equations. It is shown that homotopy perturbation method is a very fast convergent, precise and cost efficient tool for solving nonlinear problems. This homotopy perturbation method will become a much more interesting method to solving nonlinear problems in science and engineering.

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