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Variational Iteration Method for Solving Oxygen and Carbon Substrate Concentrations in Microbial Floc Particles

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Abstract

In this paper, we will extend our work in [1] on a system of two coupled nonlinear Lane-Emden differential equations, that governs the concentrations of oxygen and the carbon substrate. This mathematical model describes substrate removal, oxygen utilization and excess sludge production within a microbial floc particle as surrounded by a biodegradable substrate [1–5]. We had previously applied the Adomian decomposition method (ADM) combined with the Duan-Rach modified recursion scheme in [1], and for a comparative study, we will apply the variational iteration method (VIM) for analytical approximations of the concentrations of oxygen and the carbon substrate. The variational iteration method, as the Adomian decomposition method, yields a rapidly convergent, easily computable and readily verifiable sequence of analytic approximations that are convenient for parametric simulations.

1 Introduction

The disposal of excess sludge from waste water treatment plants represents a rising challenge in designing activated sludge processes [1–5]. Sludge comes as semi-solid material

left from waste water treatment plants, or sometimes sludge comes as solids removed from the raw water [1–5]. The sludge will become putrescent in a short time once anaerobic bacteria take over, and must be removed from the sedimentation tank before this can happen. Tyagi et al. [5] discussed the dynamic behavior of activated sludge. Abbassi et al. [2] developed a mathematical model that describes substrate removal, oxygen utilization and excess sludge production within a microbial floc particle as surrounded by a biodegradable substrate [4].

In [4], a mathematical model that relates the concentration of the carbon substrate and the concentration of oxygen was established as a system of two coupled Lane-Emden type equations

$$\frac{d^2u}{d\rho^2}+\frac{k}{\rho}\frac{du}{d\rho} = -\alpha_2+F_1\left(u(\rho),v(\rho)\right), \tag{1}$$

$$\frac{d^2v}{d\rho^2}+\frac{k}{\rho}\frac{dv}{d\rho} = F_2\left(u(\rho),v(\rho)\right). \tag{2}$$

The solution of the aforementioned system of equations requires appropriate boundary conditions. These are based on the assumption of symmetry about the floc center and neglecting the boundary layer around the floc, so that the concentration on the floc surface is equal to the concentration in the surroundings [2]. These assumptions give the two mixed sets of Neumann and Dirichlet boundary conditions

$$u'(0)=0,\ u(1)=1,\ v'(0)=0,\ v(1)=1, \tag{3}$$

where the functions $u(\rho)$ and $v(\rho)$ are the concentration of the carbon substrate and the concentration of oxygen, respectively, ρ is the radius of an idealized spherical floc particle, and the system nonlinearities are

$$F_1\left(u\left(\rho\right),v\left(\rho\right)\right) = \alpha_1 f_1\left(u\left(\rho\right),v\left(\rho\right)\right)+\alpha_3 f_2\left(u\left(\rho\right),v\left(\rho\right)\right), \tag{4}$$

$$F_2\left(u\left(\rho\right),v\left(\rho\right)\right) = \alpha_4 f_1\left(u\left(\rho\right),v\left(\rho\right)\right)+\alpha_5 f_2\left(u\left(\rho\right),v\left(\rho\right)\right), \tag{5}$$

where

$$f_1\left(u\left(\rho\right),v\left(\rho\right)\right) = \frac{u\left(\rho\right)v\left(\rho\right)}{\left(l_1+u\left(\rho\right)\right)\left(m_1+v\left(\rho\right)\right)}, \tag{6}$$

$$f_2\left(u\left(\rho\right),v\left(\rho\right)\right) = \frac{u\left(\rho\right)v\left(\rho\right)}{\left(l_2+u\left(\rho\right)\right)\left(m_2+v\left(\rho\right)\right)}, \tag{7}$$

which are products of the respective Michaelis-Menten nonlinearities [1-5], i.e.

$$f_j\left(u\left(\rho\right),v\left(\rho\right)\right)=M_j\left(u\left(\rho\right)\right)\times M_j\left(v\left(\rho\right)\right)=\frac{u\left(\rho\right)}{l_j+u\left(\rho\right)}\times\frac{v\left(\rho\right)}{m_j+v\left(\rho\right)}, \tag{8}$$

for $j = 1, 2$, where M_j is the respective Michaelis-Menten nonlinear operator. Note that in [1-5], the shape factor k was used for the specific value $k = 2$.

In our work [1], we applied the Adomian decomposition method [6–38] combined with the Duan-Rach modified recursion scheme [15–17], and we systematically obtained a rapidly convergent analytic approximate solution that is convenient for numerical simulations.

In this work, we shall apply the variational iteration method [10-12] to systematically obtain a series of successive approximations. This method mainly depends on using the correction functional scheme, where the Lagrange multipliers are necessarily needed to perform the computational work. For comparison reasons, and to enable the reader to follow our analysis, we first give a brief summary of the work in [1] which used the ADM.

2 Brief summary of the work in [1]

We rewrite Eqs. (1) and (2) in Adomian's operator-theoretic form as

$$Lu = -\alpha_2 + F_1\left(u(\rho), v(\rho)\right), \tag{9}$$

$$Lv = F_2\left(u(\rho), v(\rho)\right), \tag{10}$$

where the linear differential operator L is defined as

$$Lw(\rho) = \frac{d^2}{d\rho^2}w(\rho) + \frac{2}{\rho}\frac{d}{d\rho}w(\rho). \tag{11}$$

Defining the corresponding inverse operator L^{-1} [28, 29] as

$$L^{-1}w(\rho) = \int_0^\rho \left(r - \frac{r^2}{\rho}\right) w(r)dr, \tag{12}$$

we have [28, 29]

$$L^{-1}Lu = u\left(\rho\right) - u\left(0\right), \; L^{-1}Lv = v\left(\rho\right) - v\left(0\right), \tag{13}$$

for $\frac{du}{d\rho}\left(0\right) = 0$, and $\frac{dv}{d\rho}\left(0\right) = 0$.

Applying the corresponding inverse linear operator $L^{-1}\left(\cdot\right)$ to both sides of Eqs. (9) and (10) leads to

$$u\left(\rho\right) = u\left(0\right) - \frac{\alpha_2}{6}\rho^2 + L^{-1}F_1\left(u\left(\rho\right), v\left(\rho\right)\right), \tag{14}$$

$$v\left(\rho\right) = v\left(0\right) + L^{-1}F_2\left(u\left(\rho\right), v\left(\rho\right)\right), \tag{15}$$

which is a system of coupled nonlinear Volterra integral equations with two – as yet undetermined – constants of integration $u(0)$ and $v(0)$ as an intermediate step.

Denote

$$L_1^{-1}w(\rho) := [L^{-1}w(\rho)]_{\rho=1} = \int_0^1 \left(r - r^2\right) w(r)dr. \tag{16}$$

Substituting the boundary conditions $u(1) = 1$ and $v(1) = 1$ into Eqs. (14) and (15), we have

$$\begin{aligned} u(0) &= 1 + \frac{\alpha_2}{6} - L_1^{-1}F_1\left(u(\rho), v(\rho)\right), & (17)\\ v(0) &= 1 - L_1^{-1}F_2\left(u(\rho), v(\rho)\right). & (18) \end{aligned}$$

Substituting Eqs. (17) and (18) into Eqs. (14) and (15), we obtain the equivalent system of coupled nonlinear Fredholm-Volterra integral equations without any undetermined constants of integration as

$$\begin{aligned} u(\rho) &= 1 + \frac{\alpha_2}{6} - \frac{\alpha_2}{6}\rho^2 - L_1^{-1}F_1\left(u(\rho), v(\rho)\right) + L^{-1}F_1\left(u(\rho), v(\rho)\right), & (19)\\ v(\rho) &= 1 - L_1^{-1}F_2\left(u(\rho), v(\rho)\right) + L^{-1}F_2\left(u(\rho), v(\rho)\right). & (20) \end{aligned}$$

Next we shall use the respective Adomian decomposition series

$$u(\rho) = \sum_{n=0}^{\infty} u_n(\rho), \quad v(\rho) = \sum_{n=0}^{\infty} v_n(\rho). \tag{21}$$

Upon substitution of the decompositions (21) into Eqs. (19) and (20), we obtain

$$\sum_{n=0}^{\infty} u_n(\rho) = 1 + \frac{\alpha_2}{6} - \frac{\alpha_2}{6}\rho^2 - L_1^{-1}\sum_{n=0}^{\infty} A_{1,n}(\rho) + L^{-1}\sum_{n=0}^{\infty} A_{1,n}(\rho), \tag{22}$$

$$\sum_{n=0}^{\infty} v_n(\rho) = 1 - L_1^{-1}\sum_{n=0}^{\infty} A_{2,n}(\rho) + L^{-1}\sum_{n=0}^{\infty} A_{2,n}(\rho). \tag{23}$$

This in turn gives

$$\begin{aligned} &u_0(\rho) = 1 + \tfrac{\alpha_2}{6},\\ &u_1(\rho) = \tfrac{\alpha_2+6}{6}\left(\tfrac{\alpha_1}{(m_1+1)(\alpha_2+6l_1+6)} + \tfrac{\alpha_3}{(m_2+1)(\alpha_2+6l_2+6)}\right)(\rho^2-1) - \tfrac{\alpha_2\rho^2}{6}, \end{aligned} \tag{24}$$

and

$$\begin{aligned} &v_0(\rho) = 1,\\ &v_1(\rho) = \tfrac{\alpha_2+6}{6}\left(\tfrac{\alpha_4}{(m_1+1)(\alpha_2+6l_1+6)} + \tfrac{\alpha_5}{(m_2+1)(\alpha_2+6l_2+6)}\right)(\rho^2-1). \end{aligned}$$

The second-stage approximate solutions are therefore given as

$$\begin{aligned} \phi_2(\rho) &= u_0(\rho) + u_1(\rho),\\ &= 1 + \tfrac{\alpha_2}{6} + \tfrac{\alpha_2+6}{6}\left(\tfrac{\alpha_1}{(m_1+1)(\alpha_2+6l_1+6)} + \tfrac{\alpha_3}{(m_2+1)(\alpha_2+6l_2+6)}\right)(\rho^2-1) - \tfrac{\alpha_2\rho^2}{6}, \end{aligned} \tag{25}$$

and

$$\begin{aligned}\psi_2(\rho) &= v_0(\rho)+v_1(\rho),\\ &= 1+\tfrac{\alpha_2+6}{6}\left(\tfrac{\alpha_4}{(m_1+1)(\alpha_2+6l_1+6)}+\tfrac{\alpha_5}{(m_2+1)(\alpha_2+6l_2+6)}\right)(\rho^2-1),\end{aligned} \tag{26}$$

and so on.

3 The VIM and the Lagrange multipliers

As stated before, our concern in this work is to apply the variational iteration method to handle the system of the coupled Lane-Emden equations (1) and (2). The VIM is well documented in the literature. However, we will summarize the necessary steps of this method to allow the reader to follow our discussion in the sequel.

In this section, we will present the essential steps for using the variational iteration method and the determination of the Lagrange multipliers for various values of the shape factor k. For the differential equation

$$Lu+Nu=g(x), \tag{27}$$

where L and N are linear and nonlinear operators respectively, and $g(t)$ is the source term, a correction functional for equation (27) should be used in the form [1]

$$u_{n+1}(x)=u_n(x)+\int_0^x \lambda(x,t)\left(Lu_n(t)+N\,\tilde{\mathrm{u}}_n(t)\right)\,dt, \tag{28}$$

where $\lambda(x,t)$ is a general Lagrange multiplier, which can be a constant or a function, and can be identified optimally via the variational theory, and $\tilde{\mathrm{u}}_n$ is a restricted variation, which means that $\delta\tilde{\mathrm{u}}_n=0$.

For Eq. (1), the correction functional reads

$$u_{n+1}(x)=u_n(x)+\int_0^x \lambda(t)\left((u_n(t))_{tt}+\frac{k}{t}\,(u_n(t))_t+\tilde{\mathrm{g}}(u_n(t))\right)\,dt, \tag{29}$$

where $\delta(\tilde{\mathrm{g}}(u_n(t)))=0$.

In [11], the optimal value of $\lambda(x,t)$ was evaluated by taking the variation for both sides with respect to $u_n(x)$ to obtain

$$\delta u_{n+1}(x)=\delta u_n(x)+\delta\int_0^x \lambda(t)\left((u_n(t))_{tt}+\frac{k}{t}(u_n(t))_t+\tilde{\mathrm{g}}(u_n(t))\right)\,dt, \tag{30}$$

or equivalently

$$\delta u_{n+1}(x)=\delta u_n(x)+\delta\int_0^x \lambda(t)\left((u_n(t))_{tt}+\frac{k}{t}\,(u_n(t))_t\right)\,dt, \tag{31}$$

where we used $\delta(\tilde{g}(u_n(t))) = 0$.

Integrating the integral on the right side by parts yields

$$\begin{array}{rcl} \delta u_{n+1}(x) & = & \delta u_n(x)\left(1-\lambda^{'}(x)+\frac{k}{x}\lambda(x)\right)+\delta\lambda(x)(u_n)_t(x) \\ & + & \delta\int_0^x u_n\left(\lambda^{''}(t)-k\frac{t\lambda^{'}(t)-\lambda(t)}{t^2}\right)\,dt. \end{array} \tag{32}$$

This in turn determines the stationary conditions

$$\begin{array}{rcl} \lambda(t=x) & = & 0, \\ \lambda^{'}|_{t=x} & = & 1, \\ \lambda^{''}-k\frac{t\lambda^{'}-\lambda}{x^2} & = & 0. \end{array} \tag{33}$$

Solving (33) leads to the following two cases:

(i) For cylindrical problems, where $k = 1$, we find

$$\lambda(x,t) = t\ln\left(\frac{t}{x}\right). \tag{34}$$

(ii) For the general case, where $k > 1$, solving (33) yields

$$\lambda(x,t) = \frac{t(t^{k-1}-x^{k-1})}{(k-1)x^{k-1}}. \tag{35}$$

Recall that the shape factor $k = 2$ was used in [1-6] which describes spherical problems.

The successive approximations u_{n+1}, for $n \geq 0$, of the solution $u(x)$ will be readily obtained upon using any selective function $u_0(x)$. Consequently, the exact solution, if it exists, will be given by

$$y(x) = \lim_{n\to\infty} u_n(x). \tag{36}$$

3.1 Analysis of the problem

Our goal is to apply the variational iteration method to the model

$$\frac{d^2u}{d\rho^2}+\frac{k}{\rho}\frac{du}{d\rho} = -\alpha_2 + F_1\left(u(\rho),v(\rho)\right), \tag{37}$$

$$\frac{d^2v}{d\rho^2}+\frac{k}{\rho}\frac{dv}{d\rho} = F_2\left(u(\rho),v(\rho)\right), \tag{38}$$

subject to the two mixed sets of Neumann and Dirichlet boundary conditions

$$u'(0) = 0,\ u(1) = 1,\ v'(0) = 0,\ v(1) = 1. \tag{39}$$

To use the variational iteration method, we first determine the correction functionals in the form

$$\begin{array}{l} u_{n+1}(\rho) = u_n(\rho) \\ +\int_0^\rho \lambda(\rho,t)\left(u_n^{''}(t)+\frac{k}{t}u_n^{'}(t)+\alpha_2-F_1(u_n(t),v_n(t))\right)\,dt, \\ v_{n+1}(\rho) = v_n(\rho) \\ +\int_0^\rho \lambda(\rho,t)\left(v_n^{''}(t)+\frac{k}{t}v_n^{'}(t)-F_2(u_n(t),v_n(t))\right)\,dt. \end{array} \tag{40}$$

Recall that the Lagrange multiplier λ depends on the shape factor k which was derived earlier in (34) and (35).

It is interesting to point out that the best choice for the zeroth approximations $u_0(x)$ and $v_0(x)$, that will accelerate the convergence of the successive approximations, is the following selection

$$\begin{aligned} u_0(\rho) &= u(0) + \rho u'(0) = \alpha, \\ v_0(\rho) &= v(0) + \rho v'(0) = \beta, \end{aligned} \tag{41}$$

where the as yet undetermined constants α and β will be approximated by using the boundary conditions $u(1)$ and $v(1)$. This kind of selections has proved to be effective to achieve convergent successive approximations. Moreover, one significant feature of the VIM is that it can be applied in a straightforward manner without any restrictive assumptions such as linearity and perturbation. Also the VIM does not require the use of the Adomian polynomials. The obtained solutions for $u(x)$ and $v(x)$ will be provided in a convergent power series as proved in [10-12].

By selecting the zeroth approximation $u_0 = \alpha, v_0 = \beta$, we obtain the following calculated solution approximations for three specific values of the shape factors, namely $k = 1, k = 2$, and $k = 3$, where other cases can be evaluated in a like manner.

Case I: $k = 1$

Recall that for $k = 1$, the Lagrange multiplier is given in (34) as $\lambda(x,t) = t \ln\left(\frac{t}{x}\right)$. Using (40) we obtain the following approximations:

$$\begin{aligned} u_0(\rho) &= \alpha, \\ v_0(\rho) &= \beta, \\ u_1(\rho) &= \alpha + \left(\frac{\alpha\beta\alpha_1}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_3}{(l_2+\alpha)(m_2+\beta)} \right) \frac{\rho^2}{4} - \frac{\rho^2}{4}, \\ v_1(\rho) &= \beta + \left(\frac{\alpha\beta\alpha_4}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_5}{(l_2+\alpha)(m_2+\beta)} \right) \frac{\rho^2}{4}, \\ &\ldots. \end{aligned} \tag{42}$$

Substituting the boundary conditions $u(1) = 1$ and $v(1) = 1$ into (42) and solving the resulting equation, we can obtain the numerical values for α and β.

Case II: $k = 2$

For $k = 2$, the Lagrange multiplier is given in (35) as $\lambda(x,t) = \frac{t(t-x)}{x}$. Using (40), we obtain the following approximations:

$$\begin{aligned} u_0(\rho) &= \alpha, \\ v_0(\rho) &= \beta, \\ u_1(\rho) &= \alpha + \left(\frac{\alpha\beta\alpha_1}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_3}{(l_2+\alpha)(m_2+\beta)}\right)\frac{\rho^2}{6} - \frac{\rho^2}{6}, \\ v_1(\rho) &= \beta + \left(\frac{\alpha\beta\alpha_4}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_5}{(l_2+\alpha)(m_2+\beta)}\right)\frac{\rho^2}{6}, \\ &\ldots,. \end{aligned} \tag{43}$$

Substituting the boundary conditions $u(1) = 1$ and $v(1) = 1$ into (43) and solving the resulting equation we can obtain the numerical values for α and β.

Case III: $k = 3$

For $k = 3$, the Lagrange multiplier from (35) is given as $\lambda(x,t) = \frac{t(t^2-x^2)}{(2x^2}$. Using (40) we obtain the following approximations:

$$\begin{aligned} u_0(\rho) &= \alpha, \\ v_0(\rho) &= \beta, \\ u_1(\rho) &= \alpha + \left(\frac{\alpha\beta\alpha_1}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_3}{(l_2+\alpha)(m_2+\beta)}\right)\frac{\rho^2}{8} - \frac{\rho^2}{8}, \\ v_1(\rho) &= \beta + \left(\frac{\alpha\beta\alpha_4}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_5}{(l_2+\alpha)(m_2+\beta)}\right)\frac{\rho^2}{8}, \\ &\ldots. \end{aligned} \tag{44}$$

and this can be generalized to any k, where we obtain

$$\begin{aligned} u_0(\rho) &= \alpha, \\ v_0(\rho) &= \beta, \\ u_1(\rho) &= \alpha + \left(\frac{\alpha\beta\alpha_1}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_3}{(l_2+\alpha)(m_2+\beta)}\right)\frac{\rho^2}{2k+2} - \frac{\rho^2}{2k+2}, k \geq 1, \\ v_1(\rho) &= \beta + \left(\frac{\alpha\beta\alpha_4}{(l_1+\alpha)(m_1+\beta)} + \frac{\alpha\beta\alpha_5}{(l_2+\alpha)(m_2+\beta)}\right)\frac{\rho^2}{2k+2}, k \geq 1, \\ &\ldots. \end{aligned} \tag{45}$$

Substituting the boundary conditions $u(1) = 1$ and $v(1) = 1$ into (44) and solving the resulting equations, we can obtain the numerical values for α and β.

4 Numerical simulations

First, we assign $m_1 = l_1 = m_2 = l_2 = 0.0001$ as in [4]. We further specify α_1=5, α_2=1, α_3 =0.1, α_4=0.1, α_5=0.05 to determine the approximations for $u(\rho)$ and $v(\rho)$ for the aforementioned cases of $k = 1, 2$ and 3.

Case I: $k = 1$

Substituting the boundary conditions $u(1) = 1, v(1) = 1$ into (42) and solving the resulting equations, we find

$$\begin{array}{rcl} \alpha & = & 0.004274630305, \\ \beta & = & 0.9633610185. \end{array} \tag{46}$$

Substituting this result in (42) gives the approximations

$$\begin{array}{rcl} u_1(\rho) & = & 0.004274630305 + 0.9957253702\rho^2, \\ v_1(\rho) & = & 0.9633610185 + .03663898146\rho^2. \end{array} \tag{47}$$

Case II: $k = 2$

Substituting the boundary conditions $u(1) = 1, v(1) = 1$ into (43) and solving the resulting equations, we find

$$\begin{array}{rcl} \alpha & = & 0.3170218446, \\ \beta & = & 0.9750104464. \end{array} \tag{48}$$

Substituting this result in (43) gives the approximations

$$\begin{array}{rcl} u_1(\rho) & = & 0.3170218446 + 0.682978155\rho^2, \\ v_1(\rho) & = & 0.9750104464 + 0.02498955359\rho^2. \end{array} \tag{49}$$

It is worth noting that this approximation is consistent with our results that we obtained in [1].

Case III: $k = 3$

Substituting the boundary conditions $u(1) = 1, v(1) = 1$ into (44) and solving the resulting equations, we find

$$\begin{array}{rcl} \alpha & = & 0.8626388463, \\ \beta & = & 0.9812540837. \end{array} \tag{50}$$

Substituting this result in (44) gives the approximations

$$\begin{array}{rcl} u_1(\rho) & = & 0.8626388463 + 0.1373611537\rho^2, \\ v_1(\rho) & = & 0.9812540837 + 0.01874591629\rho^2. \end{array} \tag{51}$$

In Figs. 1 and 2 below, we plot the curves of the approximate solutions $u_1(\rho)$ and $v_1(\rho)$ for the cases $k = 1, k = 2$, and $k = 3$. Note that because the coefficient of ρ^2 is small for the three cases of $v_1(\rho)$, we observe that ρ from 0 to 1 shows that the three parabolas are almost the same for $0 \leq x \leq 1$.

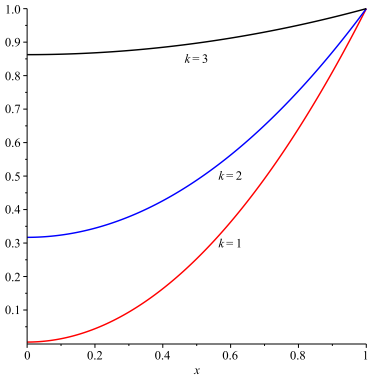

Fig. 1: Curves of the approximations $u_1(\rho)$ versus ρ for $k = 1, 2, 3$

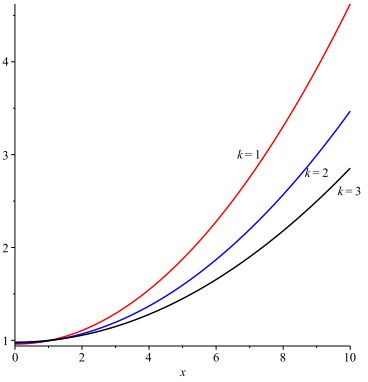

Fig. 2: Curves of the approximation $v_1(\rho)$ versus ρ for $k = 1, 2, 3$

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5 Conclusions

In this work, we have extended our results in [1] on microbial floc particles immersed in a system of the carbon substrate and oxygen. The system models the excess sludge production from waste water treatment plants. The proposed approach depends mainly on combining the variational iteration method where Lagrange multipliers are necessarily used. The work resulted in an approximation of the concentrations of carbon and the concentration of oxygen with a high level of accuracy. The evaluated approximations show consistency with respect to our previous results in [1] where the Adomian decomposition method was employed.

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