Simple stochastic model for random waste absorption of an algae cell: Analytic approach

Artorn Nokkaew , Somkid Amornsamankul, Busayamas Pimpunchat, Yaowapa Saengpayab, Wannapong Triampo

Abstract — Over the past few decades, research on water quality using biological treatment has been considerably done. The problem of how the algae dynamically absorb waste is of great important both environmental and biological science particularly concerning a problem of waste water treatment. With this regards, we have applied a model in which a Brownian agent interacts with a spin or clock in 1D to describe and predict the system of waste absorption by algae. We assumed that the waste particles executing Brownian like motion and occasionally absorbed by algae. Analytic results are presented and discussed in connection with the waste absorption by algae. It was found that the absorption nature is dominated by the exponential like nature. How this model can be improved to better understanding or match with the real system is also elaborated.

Keywords — Algae, Waste absorption, Stochastic process, Brownian.

I. Introduction

RANDOM motion has been of great interest subject for centuries. Random walks have been extensively used to study a multitude of phenomena ranging from diffusion problems to the stock market prediction [1], [2]. Brownian motion (diffusion), the motion of a particle suspended in viscous fluid resulting from fluctuating forces being the consequence of collisions with molecules of the fluid is one of the most studied problems and versatile concepts in science [3], [4], [5], [6]. Particularly to mathematicians, Brownian theory is a paradigm in stochastic processes and for myriad of applications [1], [7]. Many research works were studied concerning interacting between Brownian agent and its environment [8], [9]. A good example is the disordering agent in its environment [10], [11], [12]. Thanks to the works of the DC [10], [11], we here have proposed a new application to the environmental science problem, namely waste uptake dynamics of an algae cell. This problem may be viewed as a biological approach for a waste water treatment which here algae are treated as "water cleaner". We believe that this could be one of the green technology oriented. From physical science view point, this problem can be viewed as the problem of an interaction between an algae cell and a Brownian or random walker waste molecule.

Algae (singular alga) are a large group of diverse organisms that use photosynthesis to produce food Algae (singular alga) are a large group of diverse organisms that use photosynthesis to produce food $[http://www.wisegeek.org/what-is-algae.htm\#]$. A variety of utilization of algae has been greatly done including food [13], [14], energy [15], [16] and environment [17], [18]. Algae are important bioremediation agent that has widely being used for wastewater treatment. Waste uptakes by algae involve both adsorption and absorption [19], [20]. In the real-world system this process requires such a complicate mechanism. A number research studied capacity of algae in taking up wastes, such as phosphate, nitrogen and heavy metal [21]. Uptake capacities depend on many factors, such as size [22], waste concentration [23], [24], pH [25], [24] and etc. Moreover, uptake of waste, ammonia-N in this case, by some algae exhibited saturable kinetics. An empirical study demonstrated substrate inhibition [26]. For a late successional species, once nutrient pools in internal tissue increase exceedingly, assimilation of ammonia-N is negligible. Instead, the nutrient is stored intracellular for later assimilation. Eventually, cease of assimilation results in a decline in the uptake rate.

In this paper, the idea of Brownian motion and DC model were applied to study a problem of waste uptake by algae. Based on the model, a nutrient in intracellular pool increase via uptake process when algae interact with a bulk of waste molecules. Briefly, we shall use the one dimensional clock model or the rotating spin model, representing degrees of accumulated waste molecules in intracellular nutrient pool. The excessive amount of waste molecules in intracellular nutrient pool has negative effects on the uptake process [26]. Namely, the algae changes state from functional to inhibitory when a threshold is reached. This model consists of a Brownian waste agent (BWA) representing a waste particle moving in one dimensional space. Given the spin lying in 1D space like an array of a clock , initially all pointing in the same direction, as the BWA or waste particle meanders through the space (like stepping on the clock), it has a certain probability to rotate the spin or change the angle between the x-axis and the spin or

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clock arm direction, $\Theta(x,t)$. For the sake of simplicity, we assume that the Brownian agent (BA) is not affected by the environment in any way or no any inhomogeneity is taken into account. Hence if we start with a clock system in which all arms exist in the same state (e.g. zero $\Theta(x,t)$) or the ordered initial configuration and introduce the BA at origin $x = 0$. As time goes on, due to a random motion (Makovian process) the state or configuration of $\Theta(x,t)$ represents the "degree" of waste uptake by an algae that would be changed i.e., more likely to becoming mixture of various values of $\Theta(x,t)$ or more disordering. An interesting question concerns the degree of waste uptake by algae due to stochastic nature of the process. We have performed analytic studies using a continuum theory for a stochastic disordering process being introduced in [27] to predict how the waste absorption dynamics mediated by BWA might be using this simple stochastic model. In short, in this model the interacting between BWA and algae is studied by monitoring a dynamics of how BWA can result in the waste accumulation in algae.

The benefit from this work can be two folds. First is the theoretical viewpoint. It is of course the insight into one specific example of the stochastic process mediated by Brownian agent interacting with the rotating spin or clock in 1D. Second, it concerns an application aspect for an environmental science. Assuming the stochastic interacting between the waste particle and algae cell, this model could contribute an understanding of how the waste can dynamically be absorbed by algae.

II. Model formalism

Having adopted the model firstly proposed in DC model [10], also in [28], we briefly described as follows. The process of a Brownian agent (BA) in a two-state model is modeled on a d dimensional lattice space. Here we consider d dimension to begin with for the sake of generalization. In our application with algae, the case for $d = 3$ is the most realistic one. However, for simplicity of model analysis we focus on one dimensional problem. A position of the BA is given by a lattice vector $\overrightarrow{R}(t)$. Since here BA is a diffusing waste molecule in the water, the assumption to make the situation not very complex should be carefully applied. In the real world, water may flow or consist of other particles which may affect how the waste molecules move. Hence here we assume that no other molecule species except waste and algae molecule. In a time step δt the BA has a probability p to move to one of its $2d$ nearest neighbor sites resulting the spin or clock's arm has a probability q to change the state. The elements are described by spin variables $\sigma_{\overrightarrow{r}}$ where $\overrightarrow{r}$ denotes a discrete lattice vector. $\sigma_{\overrightarrow{r}}$ is a real number to measure the angle in the range of non-negative real number. To clarify the model we recast into the picture mapping the simplified real world situation to model world as shown in Figure 1 and Figure 2. Figure 1 depicts real world model of algae and waste particles in the water environment. Figure 2 depicts 1-dimension model of taking up waste by algae, p represents a probability of the waste particle to move to neighbor cells. q represents a probability of algae state change. $\overrightarrow{R}(t)$ and $\sigma_{\overrightarrow{r}}$ are a lattice vector of algae and a spin variable, respectively.

To describe the process, the probability distribution $P(\overrightarrow{R}, \{\sigma_{\overrightarrow{r}}\}, t)$ which is the probability that at time t, the BA is at position $\overrightarrow{R}(t)$ and the spins have values given by the set $\{\sigma_{\vec{r}}\}$. $\{\sigma_{\vec{r}}\}$ once again represent the configuration or microstate of the algae molecule. This distribution evolves according to a master equation [29] and can be given by

$$\begin{aligned} P(\overrightarrow{R}, \{\sigma_{\overrightarrow{r}}\}, t+\delta t) &= (1-p)P(\overrightarrow{R}, \{\sigma_{\overrightarrow{r}}\}, t) \\ &+ \frac{p(1-q)}{2d}\sum_{\overrightarrow{l}} P(\overrightarrow{R}+\overrightarrow{l}, \{\sigma_{\overrightarrow{r}}\}, t) \\ &+ \frac{pq}{2d}\sum_{\overrightarrow{l}} P(\overrightarrow{R}+\overrightarrow{l}, ..., -\sigma_{\overrightarrow{R}+\overrightarrow{l}}, ..., t) \end{aligned} \tag{1}$$

This equation is in principle must be solve for $P(\overrightarrow{R}, \{\sigma_{\overrightarrow{r}}\}, t)$ which contains all information of the system. One can use $P(\overrightarrow{R}, \{\sigma_{\overrightarrow{r}}\}, t)$ to various statistical values of the variables such as first or second moments. This stochastic equation is however very difficult to solve. We then take the continuum limit of this description and obtain a simple Langevin equation [12], [30]. Next, we consider the position of the BA as follows

$$\frac{d\overrightarrow{R}}{dt} = \overrightarrow{\xi}(t) \tag{2}$$

where $\overrightarrow{\xi_i}(t)$ is a white noise term, a random signal term with a flat power spectral density. Each component of this white noise is an uncorrelated Gaussian random variable with zero mean. The correlation function of $\overrightarrow{\xi_i}(t)$ is given by

$$\langle \xi_i(t)\xi_j(t') \rangle = D\delta_{i,j}\delta(t-t') \tag{3}$$

The angled brackets indicate an average over the noise. D is virtually a diffusion correlation. The evolution of the spin or continuum angle of the clock ϕ is described by

$$\partial_t \phi(\overrightarrow{r}, t) = -\lambda \phi(\overrightarrow{r}, t)\Delta_{\overrightarrow{l}}(\overrightarrow{r} - \overrightarrow{R}(t)) \tag{4}$$

Due to integrability of an equation, this equation thus may be integrated to give the explicit functional solution

$$\phi(\overrightarrow{r}, t) = exp(-\lambda \int_0^t dt' \Delta_{\overrightarrow{l}}(\overrightarrow{r} - \overrightarrow{R}(t))) \tag{5}$$

To get a particular solution, we use an initial condition $\phi(\overrightarrow{r}, 0) = 1$. It is noted the condition used here is applied for a coarse-grained sense. Next, since we want to apply the DC model to study the waste absorption due to BWA in similar to the previous works [10], [11], we then defined $\overrightarrow{\sigma}(x,t) = (cos(\Theta(x,t)), sin(\Theta(x,t))) \equiv (\sigma_1(x,t), \sigma_2(x,t))$ as spin or clock variables. Because we are interested in how the angle $\Theta(x,t)$ changes over time as BWA wandering through the space, we use the dynamics similar to that use in DC

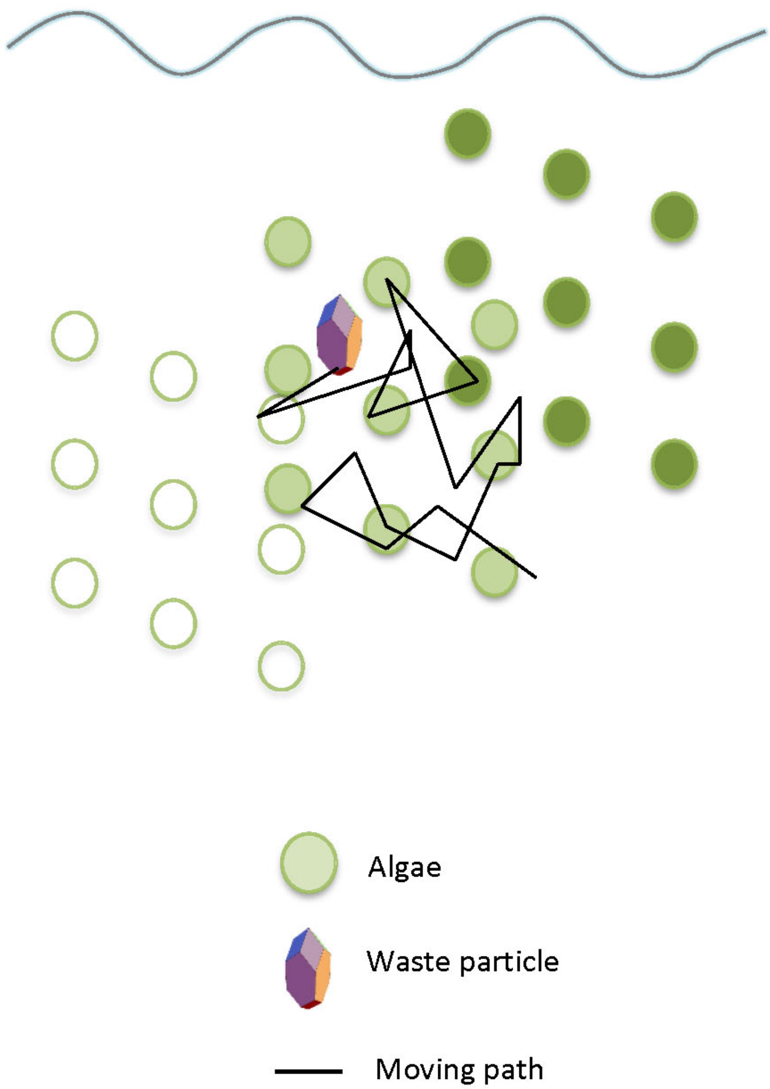


Fig. 1. Depicts real world model of algae and waste particles in the water environment.

except now the BWA interacts with the lattice by rotating the spin or clock arm as the result of changing $\Theta(x,t)$. We interpret the changes in $\Theta(x,t)$ to be equivalent to the "degree of accumulation of waste" being uptake by algae. Each time step at the waste molecule moves to where the alga is, it has a probability to be absorbed. Hence, as we can see that the time scale of the diffusing waste is much faster than that of an alga. Computationally, we write the local cellular automata to update rules for the stochastic process. For the discrete version in one dimensional space, The local update rules for this dynamic process can be written as

$$R(t+\delta t) = R(t) + l(t) \tag{6}$$

$$\Theta(x,t+\delta t) = \Theta(x,t) + \delta_{x,R(t)} \tag{7}$$

It should be noted that random motion has some different nature depending space dimension. 2D dimension is considered a critical dimension for random walk. However, this effect is not expected to play significant role on our results in connection with the real world system. Taking a continuum limit as we did before, we have for 1D situation

$$\partial_t \Theta(x,t) = \lambda \delta(x-R) \tag{8}$$

where λ is a phenomenological parameter which describes how strongly the spin or an alga is coupled to the BWA. In the real system this parameter is affected by many factors of waste particles such as mobility, affinity, temperature, waste concentration and system dimension etc. Below Figure 3 is a selected experimental result extracted from the previously published paper [26].

It is seen from the figure how the dynamics of wastes being

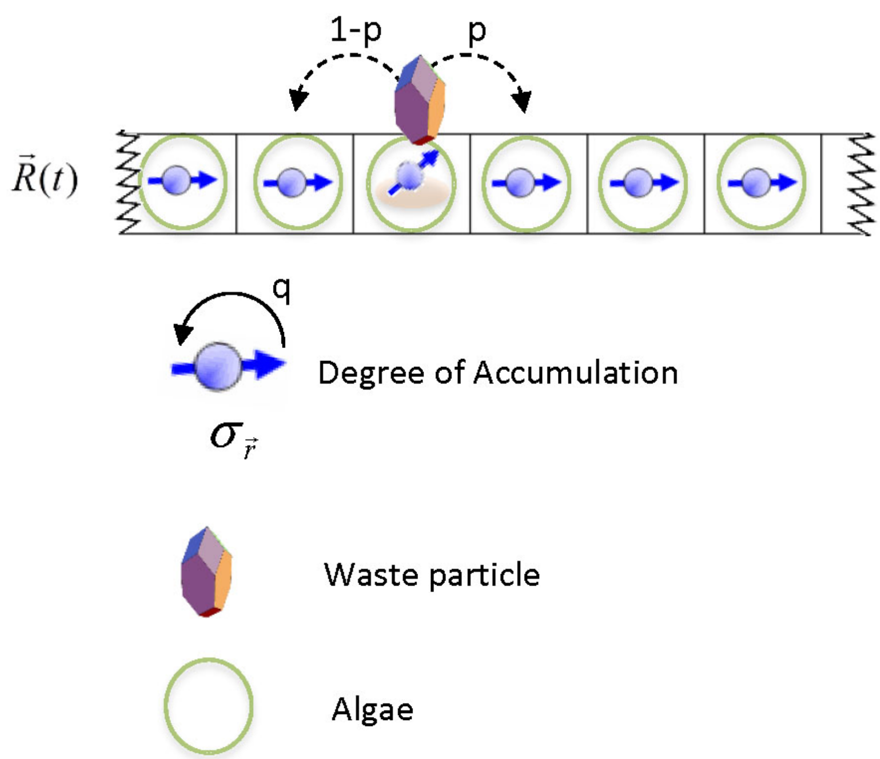


Fig. 2. Depicts 1-dimension model of taking up waste by algae.

adsorbed or up-taken by algae. We shall use this result to qualitatively compare with our analytic results from the model.

Next, we subsequently will solve and analyze the above model central to equation (8) to describe the degree of waste absorption by algae. Two and three dimension extension should be straight forward but require very tedious works.

III. Analytic results and discussion

We integrate Eq. (8), and get

$$\Theta(x,t) = \lambda \int_0^t dt' \delta(x - R(t')). \tag{9}$$

This solution requires the initial condition $\Theta(x,0) = 0$. As done in [10], [11] to get the stochastic properties that we want, we perform an average to equation (9) as follows

$$\Omega(x,t) \equiv \left\langle e^{i\Theta(x,t)} \right\rangle$$

$$= \left\langle exp\left[i\lambda \int_0^t dt' \delta(x - R(t')) \right] \right\rangle. \tag{10}$$

With some lengthy details, we thus have

$$\left\langle exp\left[-\tilde{\lambda} \int_0^t dt' \delta(x - R(t')) \right] \right\rangle = erf\left[\frac{|x|}{(2Dt)^{\frac{1}{2}}} \right]$$

$$+exp\left[\frac{\tilde{\lambda}|x|}{D} + \frac{\tilde{\lambda}^2 t}{2D} \right] erfc\left[\tilde{\lambda}\left(\frac{t}{2D} \right)^{\frac{1}{2}} + \frac{|x|}{(2Dt)^{\frac{1}{2}}} \right], \tag{11}$$

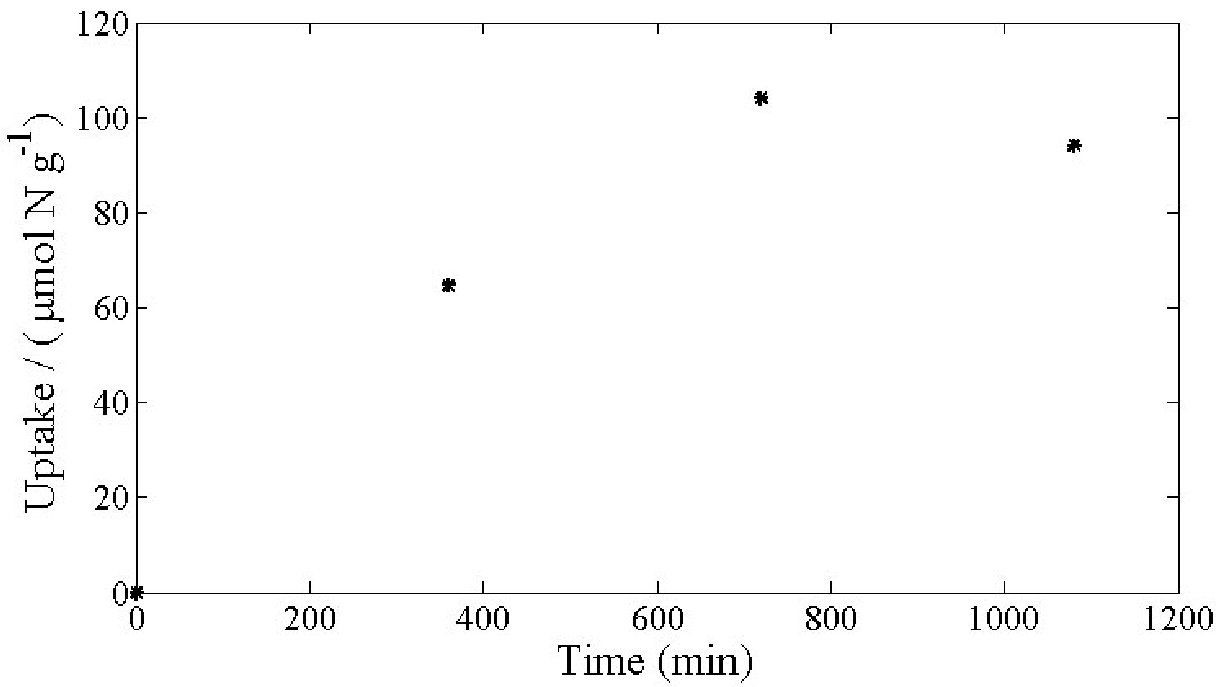


Fig. 3. The plot presents an experimental data extracted from [26].

where $\tilde{\lambda}$ is another continuum parameter, $\tilde{\lambda}$ is now $-i\lambda$ .The $\Omega(x,t)$ now takes the form

$$\Omega(x,t) = erf\left[\frac{|x|}{(2Dt)^{\frac{1}{2}}}\right] + exp\left[\frac{-i\lambda|x|}{D} - \frac{\tilde{\lambda}^2 t}{2D}\right] erfc\left[-i\lambda\left(\frac{t}{2D}\right)^{\frac{1}{2}} + \frac{|x|}{(2Dt)^{\frac{1}{2}}}\right]. \tag{12}$$

Recalling the definition of $\Omega(x,t)$, we note that

$$Re[\Omega(x,t)] = \langle cos\,(\Theta(x,t))\rangle \equiv \langle\sigma_1(x,t)\rangle \tag{13}$$

$$Im[\Omega(x,t)] = \langle sin\,(\Theta(x,t))\rangle \equiv \langle\sigma_2(x,t)\rangle \tag{14}$$

where $Re[\Omega(x,t)]$ and $Im[\Omega(x,t)]$ are the real and imaginary part of $\Omega(x,t)$ respectively.

Applying the trigonometric theorem, we get

$$\Omega(x,t) = erf\,(A) + exp\left[-\frac{\lambda^2 t}{2D}\right]\left\{cos\left(\frac{\lambda|x|}{D}\right) - isin\left(\frac{\lambda|x|}{D}\right)\right\} \left\{erfc\,(A) - B\int_0^{\lambda(\frac{t}{2D})^{1/2}} (sin(C) - icos(C))\, d\beta e^{\beta^2}\right\}, \tag{15}$$

where $A = \frac{|x|}{(2Dt)^{\frac{1}{2}}}$, $B = \frac{2}{\sqrt{\pi}}e^{-\frac{x^2}{2Dt}}$ and $C = 2\beta\frac{|x|}{(2Dt)^{\frac{1}{2}}}$.

It is a straightforward matter after some rearrangement. After more simplification, we get

$$\langle\sigma_1(x,t)\rangle = e^{-\frac{\lambda^2 t}{2D}} cos\left(\frac{\lambda|x|}{D}\right) + erf\left(\frac{|x|}{(2Dt)^{\frac{1}{2}}}\right)\left[1 - e^{-\frac{\lambda^2 t}{2D}} cos\left(\frac{\lambda|x|}{D}\right)\right] + \frac{2}{\sqrt{\pi}} exp\left(-\frac{\lambda^2 t}{2D} - \frac{x^2}{2Dt}\right) \int_0^{\lambda(\frac{t}{2D})^{1/2}} d\beta e^{\beta^2} sin\left(\frac{\lambda|x|}{D} - \frac{2\beta|x|}{(2Dt)^{\frac{1}{2}}}\right) \tag{16}$$

and

$$\langle\sigma_2(x,t)\rangle = -erfc\left(\frac{|x|}{(2Dt)^{\frac{1}{2}}}\right) e^{-\frac{\lambda^2 t}{2D}} sin\left(\frac{\lambda|x|}{D}\right) + \frac{2}{\sqrt{\pi}} exp\left(-\frac{\lambda^2 t}{2D} - \frac{x^2}{2Dt}\right) \int_0^{\lambda(\frac{t}{2D})^{1/2}} d\beta e^{\beta^2} cos\left(\frac{\lambda|x|}{D} - \frac{2\beta|x|}{(2Dt)^{\frac{1}{2}}}\right) \tag{17}$$

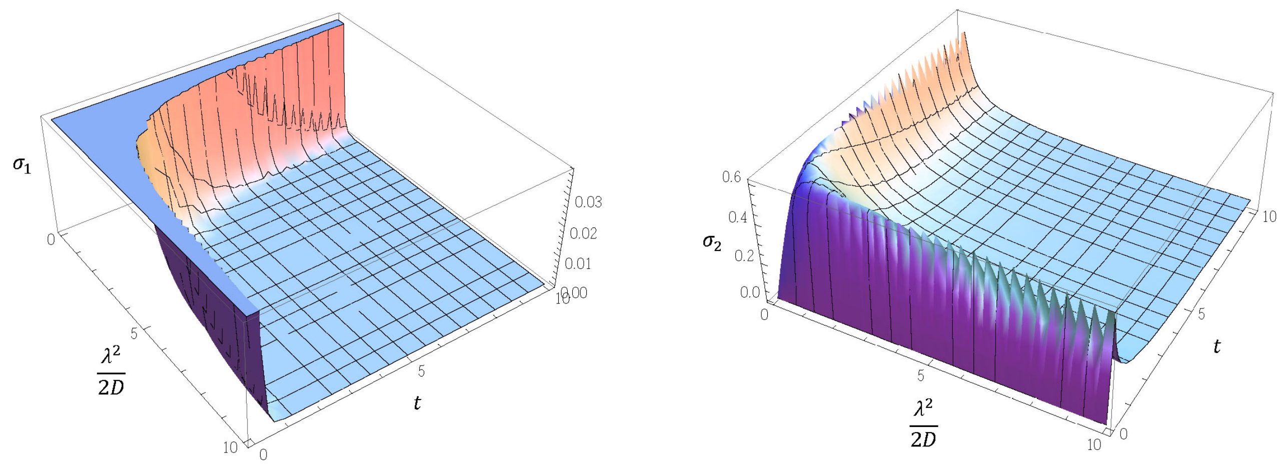
Considering the specific value of the above expression, we have, for $x = 0$,

$$\langle\sigma_1(0,t)\rangle = e^{-\frac{\lambda^2 t}{2D}}, \tag{18}$$

and

$$\langle\sigma_2(0,t)\rangle = \frac{2}{\sqrt{\pi}} e^{-\frac{\lambda^2 t}{2D}} \int_0^{\lambda\left(\frac{t}{2D}\right)^{\frac{1}{2}}} d\beta e^{\beta^2} \tag{19}$$

To see how these solutions behave, we use mathematica



(a) (b)

Fig. 4. (a) Plot of σ_1 as a function of $\frac{\lambda^2 t}{2D}$, and (b) Plot of σ_2 as a function of $\frac{\lambda^2 t}{2D}$.

software to plot equation (18) and equation (19) as shown in Figure 4(a) and Figure 4(b).

As we can see from sensitivity of the analytic function when we vary parameters that control up-take efficacy of an alga and mobility of the waste.

From the analytic results, it was found that both x and y components are dominated by and exponentially function feature. For the time evolution of x-component at $x = 0$, $\langle \sigma_1(0,t) \rangle$, it decreases exponentially to zero. While the time evolution of y-component at $x = 0$, $\langle \sigma_1(0,t) \rangle$ behaves like $\sqrt{t}$ for small times and executes $\frac{1}{\sqrt{t}}$ for large time with the maximum independent of the diffusive and the coupling constant. This indicates that as far as this model is concerned the waste is absorbed exponentially fast algae. Asymptotically, both components approach steady state. Even we here consider at $x = 0$ it still provides the same nature for other positions. Also even we consider for the infinite system case, due to length and time scales involved it would not cause any significant impact on validity of the model to explain the real world situation.

Figure 5, virtually represents the analytic result of the nutrient accumulation by an alga as predicted by the model. The graph that reflects how the degree of waste absorption by the algae changes over time provide somewhat reasonable evidence of how the model might be good enough for modeling propose. As seen from the model results, even the model is not very complicates, it does involve a great deal of fluctuation resulting non-trivial behavior since the value of variable depends sensitively on the path of the WBA interacting with the algae.

IV. Conclusion

We have applied a model in which a Brownian agent interacts with a spin or clock in 1D to investigate and predict the system of waste absorption by algae. Hence we assumed here the waste particles execute Brownian like motion. The absorption nature is dominated by the exponential like nature. This model could be validated by experimental and/or simulation data. Even this model is relative simple as a first step model, it could be modified to be more realistic in many directions. For example, one could investigate the case of the higher dimension system, many WBAs, inhomogeneous spatial system, biased or correlated motion. Hence it has yet to been how the modified version of this model can be related to the real world system.

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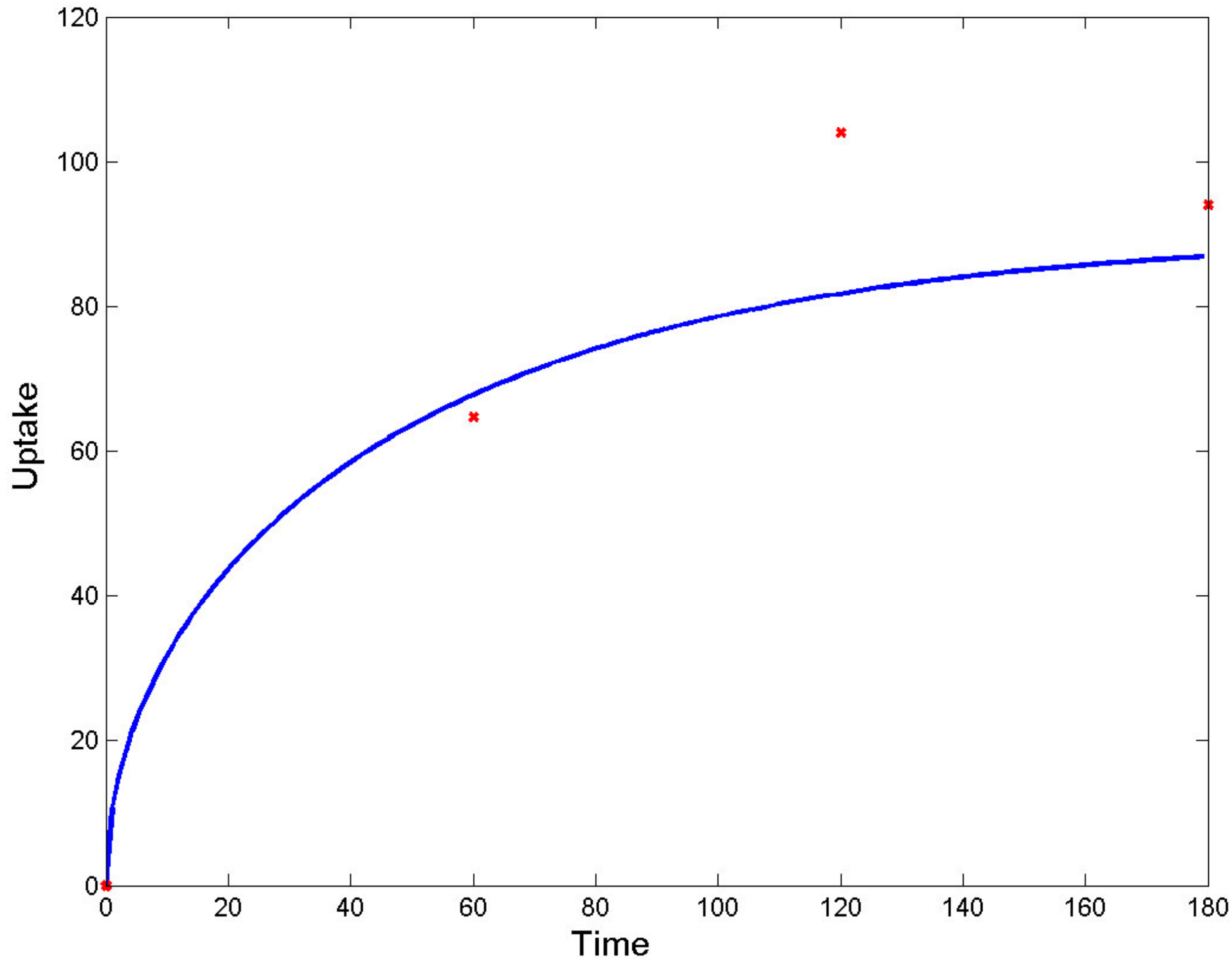

Fig. 5. Nutrient accumulation curve from analytic result.

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