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A generalized model for bacterial disinfection: Stochastic approach

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ABSTRACT

This work proposes a novel, generalized model for bacterial disinfection formulated in light of a stochastic paradigm. The model's formulation is based on an intensity of transition that is proportional to the product of general power functions of the bacteria's number concentration and time; thus, the generalized stochastic model embodies the results obtained from our earlier models. The proposed model gives rise to linear and non-linear cases of the master equation whose solution can be obtained analytically as well as numerically via Monte Carlo simulation. Moreover, the generalized stochastic model has been validated with a specific instance of bacterial disinfection. The model's analytical and numerical results are in excellent accord among themselves as well as with those obtained from our earlier models; in addition, the model's results tend to describe the available experimental data reasonably well.

1. Introduction

Mathematical models describing the behavior of bacterial populations during disinfection are ubiquitous in the available literature [1–12]. More often than not, however, these models are formulated in light of deterministic approaches that fail to quantify the incessant fluctuations of the bacterial entities being eliminated, which manifest themselves as constant variations in the experimental observations. Moreover, such fluctuations, or variations, tend to be magnified as the populations of bacteria become significantly small, thereby rendering the determination of their number concentrations uncertain or exceedingly difficult. Thus, proper quantification of these fluctuations would be essential, especially in those areas of science and industry concerned with the thorough elimination of bacteria, e.g., food safety, water treatment, or sterilization of medical equipment, whose societal impact cannot be underestimated. In this regard, it is highly desirable that a process involving bacterial entities be quantified in light of probabilistic, or stochastic, approaches, thereby incorporating the bacteria's fluctuating nature in the mathematical description of the variables characterizing the process. In fact, numerous works offer unambiguous discourses on the need for the stochastic treatment of bacterial behavior, especially the bacteria's population dynamics [13–16]. Naturally, many of these works deal with the stochastic modeling of the inactivation, or disinfection, of bacterial populations [17–20]. Nevertheless, stochastic models for bacterial disinfection based on rate expressions of generalized nature have not been available hitherto; thus, it would be plausible that the deployment of generalized rate expressions could give rise to stochastic models with superior predictive capability.

Consequently, this contribution introduces a stochastic model for bacterial disinfection whose rate expression is defined as the product of general power functions of the number concentration of bacteria and time, which exhibit powers that can be rational, positive numbers. In the parlance of the stochastic approach deployed in this work, the model's rate expression is usually termed as intensity of transition or intensity function [21,22]. Naturally, it is expected that the generalized model's performance in representing any specific set of experimental data could be enhanced in view of the flexible nature of its intensity of transition. In addition, the models developed in our earlier works [21,23,24] are embodied by the generalized stochastic model proposed herein: They presented stochastic models for bacterial disinfection each based on an intensity of transition given by the product of the first power of number concentration of bacteria and a power function of time t whose values were constrained to positive, integer numbers.

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The proposed model yields the master equation of the process under consideration, which can be linear or non-linear depending on the power of the number concentration of bacteria, i.e., the process' random variable, in the intensity of transition. Both linear and non-linear cases of the master equation can be solved analytically, thereby leading to the expressions for the mean, variance (standard deviation), and coefficient of variation of the process' random variable. On one hand, the linear cases of the master equation have been solved analytically via conventional mathematical techniques, such as the probability-generating function [22,24]. On the other hand, the difficulty in obtaining the analytical solution of the non-linear cases of the master equation has been circumvented by means of a rational approximation method, system-size expansion [22]. In this method, the process' random variable is expressed as the sum of a macroscopic term representing the mean (average) values of the process and a fluctuation term accounting for the inherent variations (fluctuations) of the process about its mean. Such a representation of the random variable gives rise to a set of differential equations whose solution yields the expressions for the process' mean and variance (standard deviation) of the non-linear cases of the master equation. For comparison, the master equation's linear and non-linear cases have also been solved numerically via simulation by resorting to the Monte Carlo method, often regarded as numerical experiments. The analytical and numerical results obtained for a set of linear cases of the generalized stochastic model have been validated by comparing them to those derived in our earlier works [21,23,24]; the comparison indicates that they are in excellent agreement. Moreover, the analytical and simulated results for a number of non-linear cases of the generalized stochastic model have been validated with the experimental observations for a specific instance of bacterial disinfection [25]. In this regard, a particular non-linear case appears to describe these experimental data more accurately than those linear cases of the generalized stochastic model equivalent to the models elaborated in two of our earlier works [23,24]. In light of these results, it is expected that the generalized stochastic model could be applied to the mathematical description of a variety of instances of bacterial disinfection performed at distinct ambient conditions and settings. Thus, the generalized stochastic model would be a valuable quantitative tool for the improvement of control strategies in areas of science and industry pivotal for human society, including microbiological risk assessment and water treatment.

2. Model formulation

The system under consideration can be modeled as a pure-death process, a particular instance of the Markovian birth-and-death process [22], as described in our earlier contributions [21,23,24]. The death event of this pure-death process is identified as the elimination of a single bacterium by means of a disinfecting agent. In addition, the process' random variable, N(t), has been defined as the number of live bacteria at time t, a realization of which is denoted by n. The states of the process are all the possible numbers of live bacteria and the state space is the collection of these numbers, $\{n_0, n_0-1, \ldots, 2, 1, 0\}$, where n_0 is the number of live bacteria present in the system at t = 0, i.e., $N(0) = n_0$.

2.1. Master equation

The master equation for the pure-death process of concern is obtained as [21–24]

$$\frac{d}{dt}p_n(t) = \mu_{n+1}(t)p_{n+1}(t) - \mu_n(t)p_n(t), \quad n = n_0, n_0-1, \ldots, 2, 1, 0 \tag{1}$$

where $p_n(t)$ signifies the probability of n live bacteria being present at time t. The master equation can be construed as a probability balance around each state n, thereby giving rise to a system of ODEs. The solution of this system yields the probability distribution, $p_n(t)$, from which the mean of the process as well as higher moments about the mean, e.g., variance or standard deviation, can be computed. For $n = n_0$, we have $\mu_{n_0+1} = 0$; thus, the above equation reduces to [21,24]

$$\frac{d}{dt}p_{n_0}(t) = -\mu_{n_0}p_{n_0}(t) \tag{2}$$

Herein, the intensity of transition (intensity of death), $\mu_n(t)$, in Eq. (1) is proposed to be of the form

$$\mu_n(t) = -\frac{dn}{dt} = k_{\alpha,\beta}n^{\alpha}t^{\beta} \tag{3}$$

where $k_{\alpha,\beta}$ is a positive constant given in the unit of $(\text{number})^{-(\alpha-1)} \times t^{-(\beta+1)}$; the powers, α and β, are rational, positive numbers, which can be other than integers. Naturally, the values of $k_{\alpha,\beta}$ as well as those of α and β depend on the nature of the bacterial strain being eliminated, or inactivated, and the disinfecting agent deployed. Substituting Eq. (3) for $\mu_n(t)$ into Eq. (1) and rearranging the resulting expression give

$$\frac{d}{dt}p_n(t) = \left[(k_{\alpha,\beta}t^{\beta})(n+1)^{\alpha}\right]p_{n+1}(t) - \left[(k_{\alpha,\beta}t^{\beta})n^{\alpha}\right]p_n(t),$$
$$n = n_0, n_0-1, \ldots, 2, 1, 0 \tag{4}$$

For $n = n_0$, we obtain

$$\frac{d}{dt}p_{n_0}(t) = -\left[(k_{\alpha,\beta}t^{\beta})n_0^{\alpha}\right]p_{n_0}(t) \tag{5}$$

Note that Eq. (4) constitutes a particular instance of the master equation for a birth-and-death process as presented by van Kampen [22], in which the coefficients accompanying n, $(k_{\alpha,\beta}t^{\beta})$'s are explicit functions of time t. According to the accepted classification in the literature [22], Eqs. (4) and (5) are linear in n, i.e., the realization of random variable N(t), only when α = 1; all other $\alpha \geq 0$ will render the same equations non-linear in n. The master equation, Eqs. (4) and (5), can be solved analytically and/or numerically for linear and non-linear cases as elaborated below.

3. Analytical solution

For the linear cases, ($\alpha = 1$, $\beta \geq 0$), the intensity of transition, $\mu_n(t)$, is obtained from Eq. (3) as

$$\mu_n(t) = -\frac{dn}{dt} = k_{1,\beta}nt^{\beta} \tag{6}$$

In light of this expression, Eqs. (4) and (5) can be rewritten, respectively, as

$$\frac{d}{dt}p_n(t) = \left[(k_{1,\beta}t^{\beta})(n+1)\right]p_{n+1}(t) - \left[(k_{1,\beta}t^{\beta})n\right]p_n(t),$$
$$n = n_0-1, \ldots, 2, 1, 0$$

and

$$\frac{d}{dt}p_{n_0}(t) = -\left[(k_{1,\beta}t^{\beta})n_0\right]p_{n_0}(t), \quad n = n_0$$

In view of their linearity, these equations can be solved analytically by means of conventional mathematical techniques, e.g., the probability-generating function [24]. By deploying the latter, the mean, m(t), of N(t) is derived as (Appendix A)

$$m_{1,\beta}(t) = n_0 \exp\left(-k_{1,\beta}\frac{t^{\beta+1}}{\beta+1}\right) \tag{7}$$