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A Non-Linear Stochastic Model for Bacterial Disinfection: Analytical Solution and Monte Carlo Simulation

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Appendix A. Derivation of the Master Equation of a Pure-Death Process

Suppose that a system comprising a population of particulate or discrete entities in a given space is to be stochastically modeled as a pure-death process. The random variable characterizing this process is denoted by N(t) with realization n; moreover, the intensity of death is denoted by $\mu_n(t)$. Thus, one of the following two events is considered to occur during time interval $(t, t+\Delta t)$. First, the number of entities decreases by one, which is a death event, with a conditional probability of $\{[\mu_n(t)]\Delta t + o(\Delta t)\}$. Second, the number of entities changes by a number other than one with a conditional probability of o(Δt), which is defined such that

$$\lim_{\Delta t \to 0} \frac{o(\Delta t)}{\Delta t} = 0 \quad \text{(A.1)}$$

Naturally, the conditional probability of no change in the number of entities during this time interval is $(1 - \{[\mu_n(t)]\Delta t + o(\Delta t)\})$.

Let the probability that exactly n entities are present at time t be denoted as $p_n(t) = \Pr[N(t) = n]$, where $n \in (n_0, n_0 - 1, ..., 2, 1, 0)$; n_0 is the initial number of entities in the system. For the two adjacent time intervals, (0, t) and $(t, t+\Delta t)$, the occurrence of exactly n entities being present at time $(t+\Delta t)$ are realized according to the following mutually exclusive events; see Figure A.1.

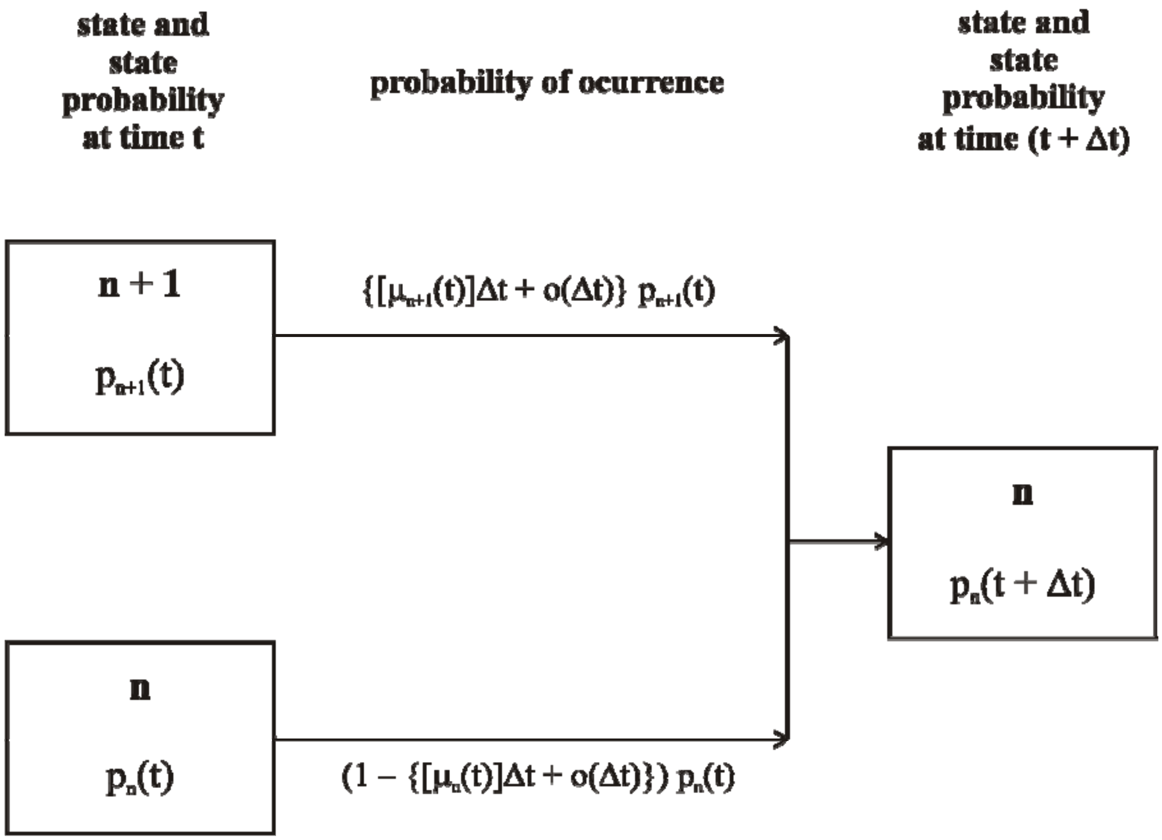

Figure A.1. Probability balance for the pure-death process involving the mutually exclusive events in the time interval, $(t, t + \Delta t)$.

(1) With a probability of $\{[\mu_{n+1}(t)]\Delta t + o(\Delta t)\}p_{n+1}(t)$, the number of entities will decrease by one during time interval $(t, t+\Delta t)$, provided that exactly $(n+1)$ entities are present at time t.

(2) With a probability of o(Δt), the number of entities will change by exactly j entities during time interval $(t, t+\Delta t)$, provided that exactly $(n-j)$ entities are present at time t, where $2 \le j \le n_0$.

(3) With a probability of $(1-\{[\mu_n(t)]\Delta t + o(\Delta t)\})p_n(t)$, the number of entities will remain unchanged during time interval $(t, t+\Delta t)$, provided that n entities are present at time t.

Summing all these probabilities and consolidating all quantities of o(Δt) yield

$$p_n(t+\Delta t) = \{[\mu_{n+1}(t)]\Delta t\}\, p_{n+1}(t) + \{1-[\mu_n(t)]\Delta t\}\, p_n(t) + o(\Delta t) \tag{A.2}$$

Rearranging this equation, dividing it by Δt, and taking the limit as Δt → 0 give rise to the master equation of the pure-death process as[1-3]

$$\frac{d}{dt}p_n(t) = \mu_{n+1}(t)\,p_{n+1}(t) - \mu_n(t)\,p_n(t) \tag{A.3}$$

This is Eq. (1) in the text. For convenience, the intensity function, $\mu_n(t)$, of the pure-death process of interest, Eq. (3) in the text, is rewritten as

$$\mu_n(t) = -\frac{dn}{dt} = knt^2 \tag{A.4}$$

Inserting the right-hand side of the above expression into the right-hand side of the master equation, Eq. (A.3), gives rise to

$$\frac{d}{dt}p_n(t) = \left[k(n+1)t^2\right]p_{n+1}(t) - \left[knt^2\right]p_n(t) \tag{A.5}$$

This is Eq. (4) in the text.

Appendix B. Derivation of the Deterministic Expression for the Number Concentration of Bacteria, y(t)

The intensity function of the pure-death process under consideration, $\mu_n(t)$, is given by Eq. (A.4) as

$$\mu_n(t) = -\frac{dn}{dt} = knt^2 \tag{B.1}$$

or

$$\frac{dn}{n} = -k\,t^2\,dt \tag{B.2}$$

By integrating both sides of this expression subject to the initial condition, $n = n_0$ at $t = t_0$, we obtain

$$\int_{n_0}^{n} \frac{dn'}{n'} = -k \int_{t_0}^{t} (t')^2\,dt'$$

or

$$\ell n\left(\frac{n}{n_0}\right) = -k\left(\frac{t^3 - t_0^3}{3}\right) \tag{B.3}$$

Solving this equation for n and denoting the resulting expression as y(t) lead to

$$y(t) = n_0 \exp\left[-k\left(\frac{t^3 - t_0^3}{2}\right)\right]$$

When $t_0 = 0$, the above equation reduces to

$$y(t) = n_0 \exp\left(-k\frac{t^3}{3}\right) \tag{B.4}$$

This is Eq. (6) in the text.

Appendix C. Derivation of the Mean and Variance for the Pure-Death Process

For convenience, the ODEs, Eqs. (4) and (5) in the text, representing the master equation of the pure-death process, are reiterated, respectively, as

$$\frac{d}{dt}p(n;t) = \left[k(n+1)t^2\right]p(n+1;t) - \left[knt^2\right]p(n;t),$$

$$n = (n_0 - 1), (n_0 - 2), ..., 2, 1, 0 \tag{C.1}$$

and

$$\frac{d}{dt}p(n_0;t) = -\left[kn_0t^2\right]p(n_0;t), \quad n = n_0 \tag{C.2}$$

where $p(n;t) = p_n(t)$ as defined in Eq. (1) in the text. This set of ODEs is subject to the following initial conditions.[2]

$$p(n;0) = \begin{cases} 0 & \text{if} \quad n = (n_0 - 1), (n_0 - 2), \ ..., 2, 1, 0 \\ 1 & \text{if} \quad n = n_0 \ , \end{cases} \tag{C.3}$$

By integrating Eq. (C.2) subject to the initial condition, $p(n_0; 0) = 1$, we obtain

$$p(n_0;t) = \exp\left(-kn_0\frac{t^3}{3}\right)$$

or

$$p(n_0;t) = \left[\exp\left(-k\frac{t^3}{3}\right)\right]^{n_0} \tag{C.4}$$

From Eq. (C.1) with $n = n_0 - 1$,

$$\frac{d}{dt}p(n_0-1;t) = \left[kn_0t^2\right]p(n_0;t) - \left[k(n_0-1)t^2\right]p(n_0-1;t)$$

Upon rearrangement,

$$\frac{d}{dt}p(n_0-1;t)+\left[k(n_0-1)t^2\right]p(n_0-1;t)=\left[kn_0t^2\right]p(n_0;t) \tag{C.5}$$

Substituting Eq. (C.4) for $p(n_0;\, t)$ into the right-hand side of this equation gives

$$\frac{d}{dt}p(n_0-1;t)+\left[k(n_0-1)t^2\right]p(n_0-1;t)=\left[kn_0t^2\right]\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{n_0} \tag{C.6}$$

Note that this expression corresponds to a first-order, linear ODE whose integrating factor, $\nu(t)$, is given by

$$\nu(t)=\exp\left\{\int_0^t\left[k(n_0-1)\tau^2\right]d\tau\right\}$$

or

$$\nu(t)=\left[\exp\left(k\frac{t^3}{3}\right)\right]^{(n_0-1)}$$

Multiplying both sides of Eq. (C.6) by this integrating factor gives rise to

$$\left[\exp\left(k\frac{t^3}{3}\right)\right]^{(n_0-1)}\frac{d}{dt}p(n_0-1;t)+p(n_0-1;t)\left[k(n_0-1)t^2\right]\left[\exp\left(k\frac{t^3}{3}\right)\right]^{(n_0-1)}$$
$$=\left[kn_0t^2\right]\exp\left(-k\frac{t^3}{3}\right)$$

or

$$\frac{d}{dt}\left\{\left[\exp\left(k\frac{t^3}{3}\right)\right]^{(n_0-1)}p(n_0-1;t)\right\}=\left[kn_0t^2\right]\exp\left(-k\frac{t^3}{3}\right)$$

Integrating this equation subject to the initial condition, $p(n_0 - 1;\, 0) = 0$, yields

$$p(n_0-1;t)=n_0\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{n_0}\left[\exp\left(k\frac{t^3}{3}\right)-1\right]$$

This expression can be rewritten as

$$p(n_0-1;t)=\frac{n_0}{1}\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{(n_0-1)}\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^1 \tag{C.7}$$

For $n = n_0 - 2$, Eq. (C.1) reduces to

$$\frac{d}{dt}p(n_0-2;t)+\left[k(n_0-2)t^2\right]p(n_0-2;t)=\left[k(n_0-1)t^2\right]p(n_0-1;t) \tag{C.8}$$

By substituting Eq. (C.7) for $p(n_0 - 1; t)$ into this equation and integrating the resulting first-order, linear ODE subject to the initial condition, $p(n_0 - 2; 0) = 0$, we have

$$p(n_0-2;t)=\frac{n_0\cdot(n_0-1)}{1\cdot 2}\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{(n_0-2)}\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^2 \tag{C.9}$$

Similarly for $n = n_0 - 3$, we obtain

$$\frac{d}{dt}p(n_0-3;t)+\left[k(n_0-3)t^2\right]p(n_0-3;t)=\left[k(n_0-2)t^2\right]p(n_0-2;t) \tag{C.10}$$

and

$$p(n_0-3;t)=\frac{n_0\cdot(n_0-1)\cdot(n_0-2)}{1\cdot 2\cdot 3}\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{(n_0-3)}\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^3 \tag{C.11}$$

Continuing by induction,

$$\begin{aligned}
p(n_0-4;t) &= \frac{n_0\cdot(n_0-1)\cdot(n_0-2)\cdot(n_0-3)}{1\cdot 2\cdot 3\cdot 4}\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{(n_0-4)}\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^4 && \text{(C.12)}\\
\vdots \quad & \vdots \qquad\qquad\qquad \vdots \\
p(n_0-m;t) &= \frac{n_0\cdot(n_0-1)\cdot(n_0-2)\cdot\ldots\cdot[n_0-(m-1)]}{1\cdot 2\cdot 3\cdot\ldots\cdot(m-1)\cdot m}\left[\exp\left(-k\frac{t^3}{3}\right)\right]^{(n_0-m)}\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^{[n_0-(n_0-m)]} && \text{(C.13)}\\
\vdots \quad & \vdots \qquad\qquad\qquad \vdots \\
p(4;t) &= \frac{n_0\cdot(n_0-1)\cdot(n_0-2)\cdot(n_0-3)\cdot(n_0-4)\ldots\cdot 6\cdot 5}{1\cdot 2\cdot 3\cdot 4\cdot 5\cdot 6\ldots\cdot(n_0-5)\cdot(n_0-4)}\left[\exp\left(-k\frac{t^3}{3}\right)\right]^4\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^{(n_0-4)}
\end{aligned}$$

Note that the above expression can be rewritten as

$$p(4;t) \quad = \quad \frac{n_0 \cdot (n_0 - 1) \cdot (n_0 - 2) \cdot (n_0 - 3)}{1 \cdot 2 \cdot 3 \cdot 4} \left[\exp\left(-k \frac{t^3}{3} \right) \right]^4 \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{(n_0 - 4)} \tag{C.14}$$

Similarly,

$$p(3;t) \quad = \quad \frac{n_0 \cdot (n_0 - 1) \cdot (n_0 - 2) \cdot (n_0 - 3) \cdot \ldots \cdot 5 \cdot 4}{1 \cdot 2 \cdot 3 \cdot 4 \cdot 5 \ldots \cdot (n_0 - 4) \cdot (n_0 - 3)} \left[\exp\left(-k \frac{t^3}{3} \right) \right]^3 \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{(n_0 - 3)}$$

or

$$p(3;t) \quad = \quad \frac{n_0 \cdot (n_0 - 1) \cdot (n_0 - 2)}{1 \cdot 2 \cdot 3} \left[\exp\left(-k \frac{t^3}{3} \right) \right]^3 \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{(n_0 - 3)} \tag{C.15}$$

and

$$p(2;t) \quad = \quad \frac{n_0 \cdot (n_0 - 1)}{1 \cdot 2} \left[\exp\left(-k \frac{t^3}{3} \right) \right]^2 \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{(n_0 - 2)} \tag{C.16}$$

$$p(1;t) \quad = \quad \frac{n_0}{1} \left[\exp\left(-k \frac{t^3}{3} \right) \right]^1 \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{(n_0 - 1)} \tag{C.17}$$

$$p(0;t) \quad = \quad \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{n_0} \tag{C.18}$$

Equations (C.4), (C.7), (C.9), and (C.11) through (C.18) collectively indicate that $p_n(t)$ or $p(n;t)$, i.e., the probability distribution of random variable $N(t)$, is given generally by

$$p(n;t) = \frac{n_0!}{n!(n_0 - n)!} \left[\exp\left(-k \frac{t^3}{3} \right) \right]^n \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]^{(n_0 - n)} \tag{C.19}$$

where

$$\frac{n_0!}{n!(n_0-n)!} = \frac{n_0 \cdot (n_0-1) \cdot (n_0-2) \cdot \ldots \cdot (n_0-n+1) \cdot (n_0-n) \cdot (n_0-n-1) \cdot \ldots \cdot 3 \cdot 2 \cdot 1}{[1 \cdot 2 \cdot 3 \cdot \ldots \cdot (n-1) \cdot n] \cdot [(n_0-n) \cdot (n_0-n-1) \cdot \ldots \cdot 3 \cdot 2 \cdot 1]}$$

$$= \frac{n_0 \cdot (n_0-1) \cdot (n_0-2) \cdot \ldots \cdot (n_0-n+1)}{[1 \cdot 2 \cdot 3 \cdot \ldots \cdot (n-1) \cdot n]}$$

Equation (C.19) can be rewritten as

$$p(n;t) = \frac{n_0!}{n!(n_0-n)!} p^n (1-p)^{(n_0-n)} \tag{C.20}$$

where

$$p = \left[\exp\left(-k\frac{t^3}{3}\right)\right] \tag{C.21}$$

In other words, N(t) obeys a binomial distribution with parameters n_0 and p, i.e., N(t) ~ Binomial(n_0, p).[4, 5] Note that the extinction probability, p(0; t), is obtained from Eq. (C.20) as

$$\begin{aligned} p(0;t) &= \frac{n_0!}{0!(n_0-0)!} p^0 (1-p)^{(n_0-0)} \\ &= (1-p)^{n_0} \end{aligned}$$

or

$$p(0;t) = \left[1-\exp\left(-k\frac{t^3}{3}\right)\right]^{n_0} \tag{C.22}$$

This expression is identical to Eq. (C.18); p(0;t) signifies the probability of the bacterial population being completely eradicated and/or inactivated at any time t.[4, 6] Clearly, p(0; t) is 0 at t = 0 and asymptotically approaches 1 as t → ∞.

In light of Eqs. (C.20) and (C.21), the mean, m(t), of random variable N(t) is obtained as[5]

$$m(t) = n_0 p$$

or

$$m(t) = n_0 \left[\exp\left(-k \frac{t^3}{3} \right) \right] \tag{C.23}$$

This is Eq. (14) in the text. Moreover, the variance, $\sigma^2(t)$, of N(t) is[5]

$$\sigma^2(t) = n_0 p (1 - p)$$

or

$$\sigma^2(t) = n_0 \left[\exp\left(-k \frac{t^3}{3} \right) \right] \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right] \tag{C.24}$$

This is Eq. (21) in the text. The standard deviation, σ(t), is the square root of the variance; thus,

$$\sigma(t) = [\sigma^2(t)]^{1/2} = n_0^{1/2} \left\{ \left[\exp\left(-k \frac{t^3}{3} \right) \right] \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right] \right\}^{1/2} \tag{C.25}$$

This is Eq. (22) in the text. In addition, the coefficient of variation, CV(t), i.e., the ratio between the standard deviation, σ(t), and the mean, m(t), is obtained from Eqs. (C.23) and (C.25) as

$$\begin{aligned} CV(t) &= \frac{\sigma(t)}{m(t)} \\ &= \frac{n_0^{1/2} \left\{ \left[\exp\left(-k \frac{t^3}{3} \right) \right] \left[1 - \exp\left(-k \frac{t^3}{3} \right) \right] \right\}^{1/2}}{n_0 \left[\exp\left(-k \frac{t^3}{3} \right) \right]} \end{aligned}$$

or

$$CV(t) = n_0^{-1/2} \left\{ \frac{\left[1 - \exp\left(-k \frac{t^3}{3} \right) \right]}{\left[\exp\left(-k \frac{t^3}{3} \right) \right]} \right\}^{1/2} \tag{C.26}$$

This is Eq. (25) in the text.

The expressions obtained above for m(t), $\sigma^2(t)$, and CV(t) can be corroborated by evaluating them via the probability generating function, G(z;t), defined as[2, 4, 7]

$$G(z;t) = \sum_n z^n p(n;t) \tag{C.27}$$

where p(n;t) = $p_n(t)$ as defined in Eq. (1) in the text, and z is an auxiliary variable. The partial derivative of this expression with respect to time t is

$$\frac{\partial}{\partial t} G(z;t) = \sum_n z^n \frac{\partial}{\partial t} p(n;t) \tag{C.28}$$

Moreover, differentiating Eq. (C.27) with respect to z gives rise to

$$\frac{\partial}{\partial z} G(z;t) = \sum_n n z^{n-1} p(n;t) \tag{C.29}$$

Multiplying both sides of this equation by z yields

$$z \frac{\partial}{\partial z} G(z;t) = \sum_n n z^n p(n;t) \tag{C.30}$$

For convenience, the set of ODEs representing the master equation of the process, Eqs. (4) and (5) in the text, is reiterated, respectively, as

$$\frac{d}{dt} p(n;t) = \left[k(n+1)t^2\right] p(n+1;t) - \left[knt^2\right] p(n;t),$$

$$n = (n_0 - 1), (n_0 - 2), ..., 2, 1, 0 \tag{C.31}$$

and

$$\frac{d}{dt} p(n_0;t) = -\left[k n_0 t^2\right] p(n_0;t), \quad n = n_0 \tag{C.32}$$

By multiplying both sides of Eq. (C.31) by the respective z^n's and both sides of Eq. (C.32) by z^{n_0}, we have

$$
\begin{aligned}
z^0 \frac{d}{dt} p(0;t) &= \left[k(1)t^2\right] z^0 p(1;t) - \overbrace{\left[k(0)t^2\right]}^{=0} z^0 p(1;t) \\
z^1 \frac{d}{dt} p(1;t) &= \left[k(2)t^2\right] z^1 p(2;t) - \left[k(1)t^2\right] z^1 p(1;t) \\
z^2 \frac{d}{dt} p(2;t) &= \left[k(3)t^2\right] z^2 p(3;t) - \left[k(2)t^2\right] z^2 p(2;t) \\
\vdots \qquad & \vdots \qquad \vdots \qquad \vdots \qquad \vdots
\end{aligned}
$$

$$
\begin{aligned}
\vdots \qquad & \vdots \qquad \vdots \qquad \vdots \qquad \vdots \\
z^{(n_0-2)} \frac{d}{dt} p(n_0-2;t) &= \left[k(n_0-1)t^2\right] z^{(n_0-2)} p(n_0-1;t) - \left[k(n_0-2)t^2\right] z^{(n_0-2)} p(n_0-2;t) \\
z^{(n_0-1)} \frac{d}{dt} p(n_0-1;t) &= \left[k(n_0)t^2\right] z^{(n_0-1)} p(n_0;t) - \left[k(n_0-1)t^2\right] z^{(n_0-1)} p(n_0-1;t) \\
z^{n_0} \frac{d}{dt} p(n_0;t) &= \left[k(n_0+1)t^2\right] z^{(n_0)} \underbrace{p(n_0+1;t)}_{=0} - \left[k(n_0)t^2\right] z^{n_0} p(n_0;t)
\end{aligned}
$$

Summing all these equations gives

$$
\begin{aligned}
& z^{n_0} \frac{d}{dt} p(n_0;t) + z^{(n_0-1)} \frac{d}{dt} p(n_0-1;t) + z^{(n_0-2)} \frac{d}{dt} p(n_0-2;t) \\
& \quad + \cdots + z^2 \frac{d}{dt} p(2;t) + z^1 \frac{d}{dt} p(1;t) + z^0 \frac{d}{dt} p(0;t) \\
& = (kt^2)\Big[0 + (n_0) z^{(n_0-1)} p(n_0;t) + (n_0-1) z^{(n_0-2)} p(n_0-1;t) \\
& \quad + \cdots + (3) z^2 p(3;t) + (2) z^1 p(2;t) + (1) z^0 p(1;t)\Big] \\
& \quad - (kt^2)\Big[(n_0) z^{n_0} p(n_0;t) + (n_0-1) z^{(n_0-1)} p(n_0-1;t) \\
& \quad + (n_0-2) z^{(n_0-2)} p(n_0-2;t) + \cdots + (2) z^2 p(2;t) + (1) z^1 p(1;t) + 0\Big]
\end{aligned}
$$

or

$$
\sum_{n=n_0}^{0} z^n \frac{d}{dt} p(n;t) = (kt^2) \sum_{n=n_0}^{0} n z^{n-1} p(n;t) - (kt^2) \sum_{n=n_0}^{0} n z^n p(n;t) \tag{C.33}
$$

In view of Eqs. (C.27) through (C.30), this expression can be rewritten as

$$
\frac{\partial}{\partial t} G(z;t) = (kt^2)\left[\frac{\partial}{\partial z} G(z;t) - z \frac{\partial}{\partial z} G(z;t)\right]
$$

or

$$\frac{\partial}{\partial t}G(z;t) = (kt^2)(1-z)\frac{\partial}{\partial z}G(z;t) \tag{C.34}$$

For the pure-death process under consideration,[2]

$$p(n;0) = \begin{cases} 0 & \text{if} \quad n = (n_0 - 1), (n_0 - 2), \ ..., 2, 1, 0 \\ \\ 1 & \text{if} \quad n = n_0 \ , \end{cases} \tag{C.35}$$

In light of this set of initial conditions, we obtain, from Eq. (C.27),

$$\begin{aligned} G(z;0) &= \sum_{n=n_0}^{0} z^n p(n;0) \\ &= z^{n_0} p(n_0;0) + z^{(n_0-1)} p(n_0 - 1;0) + z^{(n_0-2)} p(n_0 - 2;0) \\ &\quad + \cdots + z^2 p(2;0) + z^1 p(1;0) + z^0 p(0;0) \end{aligned}$$

or

$$G(z;0) = z^{n_0} \tag{C.36}$$

Moreover,

$$\begin{aligned} G(1;t) &= \sum_{n=n_0}^{0} (1)^n p(n;t) \\ &= \sum_{n=n_0}^{0} p(n;t) \end{aligned}$$

or

$$G(1;t) = 1 \tag{C.37}$$

The partial differential equation (PDE) in terms of G(z;t), Eq. (C.34), can be solved by resorting to the method of characteristics[8](REF) with the initial condition given by Eq. (C.36). In this method, the PDE in terms of G(z;t) is reduced to a set of ODEs along characteristic curves [z(r), t(r)] where r is a parameterization variable. The solution of the original PDE is evaluated by solving the parameterized set of ODEs; its form will be dictated by the initial condition. For the case under consideration,

$$G(z;t) = G\left[z(r);t(r)\right]$$

From this equation,

$$\frac{d}{dr}G(z;t) = \left(\frac{dz}{dr}\right)\frac{\partial}{\partial z}G(z;t) + \left(\frac{dt}{dr}\right)\frac{\partial}{\partial t}G(z;t) \tag{C.38}$$

Rearranging Eq. (C.34) gives rise to

$$0 = (kt^2)(1-z)\frac{\partial}{\partial z}G(z;t) - \frac{\partial}{\partial t}G(z;t) \tag{C.39}$$

By comparing the respective terms in both sides of Eqs. (C.38) and (C.39),

$$\frac{dt}{dr} = -1, \tag{C.40}$$

$$\frac{dz}{dr} = (kt^2)(1-z), \tag{C.41}$$

and

$$\frac{d}{dr}G(z;t) = 0 \tag{C.42}$$

These ODEs can be solved by assuming that $r = 0$ and $z = z_0$ at $t = 0$. From Eq. (C.40), therefore,

$$t = -r \tag{C.43}$$

Owing to this equation, Eq. (C.41) can be rewritten as

$$-\frac{dz}{dt} = (kt^2)(1-z)$$

or

$$\frac{dz}{(1-z)} = -(kt^2)dt$$

Upon integration,

$$(1-z)^{-1} = c_1 \exp\left(-k\frac{t^3}{3}\right) \tag{C.44}$$

Because $z = z_0$ at $t = 0$,

$$c_1 = (1-z_0)^{-1}$$

Hence, Eq. (C.44) becomes

$$(1-z)^{-1} = (1-z_0)^{-1} \exp\left(-k\frac{t^3}{3}\right)$$

Solving this equation for z_0 yields

$$z_0 = 1-(1-z)\exp\left(-k\frac{t^3}{3}\right) \tag{C.45}$$

Integrating Eq. (C.42) results in

$$G(z;t) = \text{ constant} \tag{C.46}$$

In other words, $G(z, t)$ is constant along the characteristic curve whose form depends on the initial condition, $z = z_0$ at $t = 0$; as a result,

$$G(z;t) = \text{constant} = G(z_0, 0) \tag{C.47}$$

From, Eq. (C.36),

$$G(z_0;0) = z_0^{n_0} \tag{C.48}$$

Consequently,

$$G(z;t) = z_0^{n_0}$$

Substituting Eq. (C.45) into the above expression leads to

$$G(z;t) = \left[1-(1-z)\exp\left(-k\frac{t^3}{3}\right)\right]^{n_0} \tag{C.49}$$

or

$$G(z;t) = \left[1 - (1-z)\,p\right]^{n_0} \tag{C.50}$$

where

$$p = \left[\exp\left(-k\frac{t^3}{3}\right)\right] \tag{C.51}$$

By rearranging Eq. (C.50), we have

$$G(z;t) = \left[(1-p) + z\,p\right]^{n_0} \tag{C.52}$$

This expression is identified as the probability generating function of a binomial distribution with parameters n_0 and *p*.[9] The expression yields G(1; t) = 1, thereby ascertaining that it also satisfies the boundary condition given by Eq. (C.37).

The mean, E[N(t)] or m(t), of random variable N(t) is defined as[2, 10]

$$E[N(t)] = m(t) = \sum_n np(n;t) \tag{C.53}$$

From the definition of G(z;t), given by Eq. (C.27),

$$\frac{\partial}{\partial z}G(z;t) = \sum_n nz^{n-1}p(n;t)$$

This is Eq. (C.29) derived earlier. Evaluating this expression at z = 1 yields

$$\left.\frac{\partial}{\partial z}G(z;t)\right|_{z=1} = \sum_n np(n;t)$$

From the definition of mean given in Eq. (C.53),

$$\left.\frac{\partial}{\partial z}G(z;t)\right|_{z=1} = E[N(t)] = m(t) \tag{C.54}$$

For the process under consideration, the partial derivative of G(z;t) with respect to z is obtained from Eq. (C.52) as

$$\frac{\partial}{\partial z}G(z;t) = n_0\left[(1-p)+zp\right]^{n_0-1}p$$

Therefore,

$$\left.\frac{\partial}{\partial z}G(z;t)\right|_{z=1} = m(t) = n_0 p \qquad (C.55)$$

Consequently, in light of Eq. (C.51),

$$m(t) = n_0 \exp\left(-k\frac{t^3}{3}\right) \qquad (C.56)$$

Note that this expression is identical to Eq. (C.23).

The variance, Var[N(t)] or $\sigma^2(t)$, of random variable N(t) is defined as[2, 10]

$$\mathrm{Var}[N(t)] = \sigma^2(t) = \sum_n \{n - E[N(t)]\}^2 p(n;t) \qquad (C.57)$$

By expanding the right-hand side of this expression, we obtain

$$\mathrm{Var}[N(t)] = \sum_n n^2 p(n;t) - 2E[N(t)]\underbrace{\sum_n np(n;t)}_{=E[N(t)]} + \{E[N(t)]\}^2\overbrace{\sum_n p(n;t)}^{=1}$$

or

$$\sigma^2(t) = E[N^2(t)] - [m(t)]^2 \qquad (C.58)$$

where

$$E[N^2(t)] = \sum_n n^2 p(n;t) \qquad (C.59)$$

From the definition of G(z;t), given by Eq. (C.27),

$$\frac{\partial^2}{\partial z^2} G(z;t) = \sum_n n(n-1) z^{n-2} p(n;t)$$

Evaluating this expression at z = 1 yields

$$\left.\frac{\partial^2}{\partial z^2} G(z;t)\right|_{z=1} = \sum_n n^2 p(n;t) - \sum_n np(n;t)$$

In view of Eqs. (C.53) and (C.59), this equation reduces to

$$\left.\frac{\partial^2}{\partial z^2} G(z;t)\right|_{z=1} = E[N^2(t)] - m(t) \tag{C.60}$$

Thus,

$$E[N^2(t)] = \left[\left.\frac{\partial^2}{\partial z^2} G(z;t)\right|_{z=1}\right] + m(t) \tag{C.61}$$

Substituting the above equation into Eq. (C.58) gives rise to

$$\sigma^2(t) = \left[\left.\frac{\partial^2}{\partial z^2} G(z;t)\right|_{z=1}\right] + m(t) - [m(t)]^2 \tag{C.62}$$

For the process under consideration, the second partial derivative of G(z;t) with respect to z is obtained from Eq. (C.52) as

$$\frac{\partial^2}{\partial z^2} G(z;t) = n_0(n_0-1)\left[(1-p) + zp\right]^{n_0-2} p^2$$

Thus,

$$\left.\frac{\partial^2}{\partial z^2} G(z;t)\right|_{z=1} = n_0(n_0-1)p^2 \tag{C.63}$$

By substituting Eqs. (C.55) and (C.63) into the right-hand side of Eq. (C.62), we obtain

$$\sigma^2(t) = n_0(n_0-1)p^2 + n_0 p - (n_0 p)^2$$

or

$$\sigma^2(t) = n_0 p(1-p) \tag{C.64}$$

In light of Eq. (C.51),

$$\sigma^2(t) = n_0\left[\exp\left(-k\frac{t^3}{3}\right)\right]\left[1-\exp\left(-k\frac{t^3}{3}\right)\right] \tag{C.65}$$

Note that this expression is identical to Eq. (C.24). From this equation, the standard deviation, $\sigma(t)$, is

$$\sigma(t) = [\sigma^2(t)]^{1/2} = n_0^{1/2}\left\{\left[\exp\left(-k\frac{t^3}{3}\right)\right]\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]\right\}^{1/2} \tag{C.66}$$

This expression is identical to Eq. (C.25). From Eqs. (C.56) and (C.66), the coefficient of variation, CV(t), is

$$CV(t) = \frac{\sigma(t)}{m(t)} = \frac{1}{n_0^{1/2}}\left\{\frac{\left[1-\exp\left(-k\frac{t^3}{3}\right)\right]}{\left[\exp\left(-k\frac{t^3}{3}\right)\right]}\right\}^{1/2}$$

This expression is identical to Eq. (C.26).

Appendix D. Derivation of the Probability Density Function and the Cumulative Distribution Function of Waiting Time for the Pure-Death Process

Let T_n be a random variable representing the waiting time between events for the pure-death process of interest with the intensity of death, $\mu_n(t)$; a realization of T_n is denoted by τ. Given that it is in state n at time t, the system is assumed to remain in this state during time interval $(t, t+\tau)$ at the end of which, i.e., at $(t+\tau)$, a transition occurs and the state of the system changes. The probability that a transition occurs during time interval $(t, t+\tau)$ is specified by the cumulative distribution function, cdf, of T_n with realization τ. This function is denoted by $H_n(\tau)$ and defined as[11]

$$H_n(\tau) = \Pr[T_n \le \tau] \tag{D.1}$$

By definition, $H_n(\tau)$ ranges from 0 to 1. Moreover, the probability that no transition occurs during time interval $(t, t+\tau)$ given that the system is in state n at time t, $G_n(\tau)$, is defined as[11]

$$G_n(\tau) = \Pr[T_n > \tau] = 1 - H_n(\tau) \tag{D.2}$$

For the succeeding small time interval $[(t+\tau), (t+\tau)+\Delta\tau]$,[10, 12]

$$H_n(\Delta\tau) = [\mu_n(t+\tau)]\Delta\tau + o(\Delta\tau) \tag{D.3}$$

where $o(\Delta\tau)$ is defined such that

$$\ell\mathrm{im}_{\Delta\nu \to 0} \frac{o(\Delta\tau)}{\Delta\tau} = 0,$$

Note that the intensity of death, $\mu_n(t)$, in Eq. (D.3) is evaluated at the time at which a transition occurs, i.e., at $(t+\tau)$. On the basis of Eq. (D.2), we obtain

$$G_n(\Delta\tau) = \{1 - [\mu_n(t+\tau)]\Delta\tau\} + o(\Delta\tau) \tag{D.4}$$

The Markovian property implies that disjoint time intervals are independent of one another; thus,[11]

$$G_n(\tau+\Delta\tau) = G_n(\tau) G_n(\Delta\tau) \tag{D.5}$$

Inserting Eq. (D.4) into the above equation results in

$$G_n(\tau+\Delta\tau) = G_n(\tau)\{1-[\mu_n(t+\tau)]\Delta\tau\} + o(\Delta\tau) \tag{D.6}$$

Expanding and rearranging this expression yield

$$G_n(\tau+\Delta\tau) - G_n(\tau) = -[\mu_n(t+\tau)] G_n(\tau)\Delta\tau + o(\Delta\tau) \tag{D.7}$$

Dividing both sides of this equation by $\Delta\tau$ and taking the limit as $\Delta\tau \to 0$ give rise to

$$\frac{d}{d\tau} G_n(\tau) = -[\mu_n(t+\tau)] G_n(\tau) \tag{D.8}$$

By integrating this ordinary differential equation subject to the initial condition,[11-13]

$$G_n(0) = 1,$$

we have

$$G_n(\tau) = \exp\left\{-\int_0^{\tau} [\mu_n(t+\tau')] d\tau'\right\} \tag{D.9}$$

Equation (D.2) in conjunction with the above equation lead to

$$H_n(\tau) = 1 - \exp\left\{-\int_0^{\tau} [\mu_n(t+\tau')] d\tau'\right\} \tag{D.10}$$

Differentiating both sides of this equation with respect to τ gives

$$\frac{d}{d\tau} H_n(\tau) = [\mu_n(t+\tau)] \exp\left\{-\int_0^{\tau} [\mu_n(t+\tau')] d\tau'\right\} \tag{D.11}$$

The probability density function, pdf, of T_n given that the system is in state n at time t, $h_n(\tau)$, is defined as

$$h_n(\tau) = \frac{d}{d\tau} H_n(\tau) \tag{D.12}$$

Naturally,

$$H_n(\tau) = \int_0^{\tau} h_n(\tau')\, d\tau' \tag{D.13}$$

In light of Eq. (D.12), Eq. (D.11) can be rewritten as

$$h_n(\tau) = [\mu_n(t+\tau)] \exp\left\{ -\int_0^{\tau} [\mu_n(t+\tau')] d\tau' \right\} \tag{D.14}$$

The above equation and Eq. (D.10) collectively reveal that the pdf of T_n is exponential.[10, 12] Clearly, the parameter of this pdf depends on the form of the intensity of death, $\mu_n(t)$. Inserting Eq. (3) in the text for $\mu_n(t)$ into Eq. (D.10) yields

$$H_n(\tau) = 1 - \exp\left\{ -\int_0^{\tau} [kn(t+\tau')^2] d\tau' \right\} \tag{D.15}$$

Integrating this expression gives rise to

$$H_n(\tau) = 1 - \exp\left\{ -kn\left[\frac{(t+\tau)^3 - t^3}{3} \right] \right\} \tag{D.16}$$

In light of Eq. (D.12),

$$h_n(\tau) = [kn(t+\tau)^2] \exp\left\{ -kn\left[\frac{(t+\tau)^3 - t^3}{3} \right] \right\} \tag{D.17}$$

These two equations indicate that the pdf of random variable T_n is exponential with parameter $[kn(t+\tau)]$, i.e., the intensity of death at time $(t+\tau)$, $\mu_n(t+\tau)$, of the pure-death process of concern, which is dependent on realization n and time t.

Appendix E. Estimation of Waiting Time for the Pure-Death Process

As indicated in the preceding appendix, the random variable, T_n, with realization τ represents the waiting time between successive events for a pure-death process. Equation (C.27) repeated below defines $H_n(\tau)$, i.e., the cdf of T_n, as

$$H_n(\tau) = \Pr[T_n \le \tau] \tag{E.1}$$

This cdf signifies the probability that the system undergoes a transition during time interval $(t, t+\tau)$ given that it is in state n at time t.

Let U be a random variable defined as

$$U = H_n(T_n) \tag{E.2}$$

Thus, u, which is a realization of U, is

$$u = H_n(\tau) \tag{E.3}$$

By definition, any realization u is within the range from 0 to 1. Naturally, the cdf of U with realization u, i.e., $F_U(u)$, is given by

$$F_U(u) = \Pr[U \le u] \tag{E.4}$$

In light of Eqs. (E.2) and (E.3), the above expression becomes

$$F_U(u) = \Pr[H_n(T_n) \le H_n(\tau)] \tag{E.5}$$

The inverse function of any given function, $y = f(x)$, is defined as $x = f^{-1}(y)$, or $x = f^{-1}[f(x)]$, provided that f(x) is continuous and strictly increasing.[8] In other words, the inverse function, $x = f^{-1}(y)$, reverses what the original function, $y = f(x)$, performs over any value x of its domain, thereby returning x. Note that the inverse function of f(x) is not its reciprocal or multiplicative inverse, which is given by [1/f(x)] or $[f(x)]^{-1}$. Herein, $y = f(x)$ stands for U = $H_n(T_n)$ on the basis of Eq. (E.2); thus, the inverse function of U is given by

$$T_n = H_n^{-1}(U)$$

Substituting Eq. (E.2) in the right-hand side of the above equation yields

$$T_n = H_n^{-1}[H_n(T_n)] \tag{E.6}$$

and therefore,

$$\tau = H_n^{-1}[H_n(\tau)] \tag{E.7}$$

Given that the functions, $H_n(T_n)$ and $H_n(\tau)$, are continuous and strictly increasing, they can be substituted by $H_n^{-1}[H_n(T_n)]$ and $H_n^{-1}[H_n(\tau)]$, respectively, in the inequality within the bracket on the right-hand side of Eq. (E.5) without altering the inequality;[5] hence,

$$F_U(u) = \Pr\left\{H_n^{-1}[H_n(T_n)] \le H_n^{-1}[H_n(\tau)]\right\} \tag{E.8}$$

In view of Eqs. (E.6) and (E.7), this equation reduces to

$$F_U(u) = \Pr[T_n \le \tau] \tag{E.9}$$

Note that the right-hand side of this expression is $H_n(\tau)$ as defined by Eq. (E.1); thus,

$$F_U(u) = H_n(\tau) \tag{E.10}$$

Because of Eq. (E.3),

$$F_U(u) = u \tag{E.11}$$

This is the expression for the cdf of U with realization u; by definition, its pdf is

$$f_U(u) = \frac{d}{du} F_U(u)$$

Substituting Eq. (E.11) into the right-hand side of the above equation gives

$$f_U(u) = \frac{d}{du}(u)$$

or

$$f_U(u) = 1 \tag{E.12}$$

This equation in conjunction with Eq. (E.11) imply that U is the uniform random variable on interval (0, 1).[5] As a result, a realization of T_n, i.e., τ, can be estimated by sampling a realization of U, i.e., u, on interval (0, 1), and solving Eq. (E.3) for τ as[10]

$$\tau = H_n^{-1}(u) \tag{E.13}$$

Figure E.1 illustrates this estimation of waiting time τ. For convenience, Eq. (E.3) is rewritten below as

$$u = H_n(\tau) \tag{E.14}$$

For the pure-death process of concern, the expression for $H_n(\tau)$ is given by Eq. (D.16) as

$$H_n(\tau) = 1 - \exp\left\{-kn\left[\frac{(t+\tau)^3 - t^3}{3}\right]\right\}$$

Inserting the above expression into the right-hand side of Eq. (E.14) gives rise to

$$u = 1 - \exp\left\{-kn\left[\frac{(t+\tau)^3 - t^3}{3}\right]\right\}$$

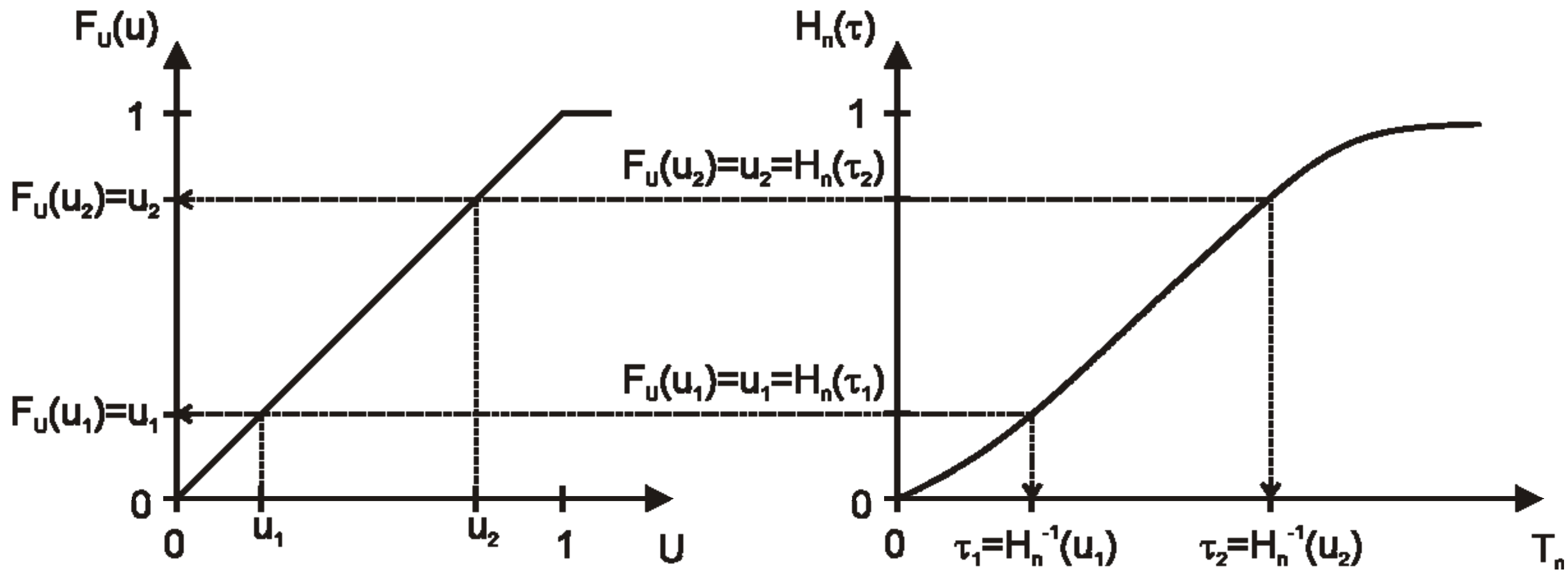

Figure E.1. Schematic for estimating realization τ of the random variable, T_n, representing the waiting time on the basis of realization u of the uniform random variable, U, on interval (0,1).

By solving the above expression for τ, we have

$$\tau = -t + \left[t^3 - \frac{3}{kn} \ell n(1-u) \right]^{\frac{1}{3}} \tag{E.15}$$

This is Eq. (31) in the text; note that τ is dependent on both realization n and time t. Because $t \geq 0$, $u \in [0, 1)$ and $\ell n(1 - u) < 0$, τ estimated from this equation is positive, and thus, physically significant, provided that $k > 0$ and $n > 0$.

Appendix F. Procedure to Implement the Monte Carlo Method via the Event-driven Approach for the Pure-Death Process

The master equation of the pure-death process is simulated by resorting to the Monte Carlo method via the event-driven approach by executing the following sequence of steps.

Step 1. Define the initial number of bacteria, n_0, the total number of simulations, Z_f, and the length of each simulation, t_f. Initialize the simulation counter as $Z \leftarrow 1$.

Step 2. Initialize clock time t, data-recording time θ,[14] the realization of N(t) at time t for simulation Z, $n_Z(t)$, and the realization of N(θ) at time θ for simulation Z, $n_Z(\theta)$, as follows:

$$t \leftarrow t_0$$

$$\theta_0 \leftarrow t_0$$

$$n_Z(t_0) \leftarrow n_0$$

$$n_Z(\theta_0) \leftarrow n_Z(t_0)$$

Step 3. Sample a realization u from the uniform random variable, U, on interval [0, 1). Estimate a realization τ of random variable T_n representing the waiting time between successive death events according to the following expression (see Appendix E);

$$\tau = -t + \left[t^3 - \frac{3}{kn} \ell n(1-u) \right]^{\frac{1}{3}}$$

where $n = n_Z(t)$.

Step 4. Advance clock time as $t \leftarrow (t + \tau)$.

Step 5. If ($\theta < t$), then go to the next step; otherwise, go to Step 8.

Step 6. Compute the sample mean, variance, and standard deviation at time θ as follows:

a. Record the value of realization at θ, $n_Z(\theta)$:

$$n_Z(\theta) \leftarrow n_Z(t-\tau)$$

b. Store the sum of realizations at θ:

$$\Xi_Z(\theta) \leftarrow \sum_{Z=1}^{Z} n_Z(\theta)$$

c. Store the sum of squares of realizations at θ:

$$\Phi_Z(\theta) \leftarrow \sum_{Z=1}^{Z} n_Z^2(\theta)$$

d. Store the square of sum of realizations at θ:

$$\Psi_Z(\theta) \leftarrow \left[\sum_{Z=1}^{Z} n_Z(\theta)\right]^2 = [\Xi_Z(\theta)]^2$$

e. Compute the sample mean at θ:[12, 15]

$$m_Z(\theta) \leftarrow \frac{1}{Z}\sum_{Z=1}^{Z} n_Z(\theta) = \frac{1}{Z}\Xi_Z(\theta)$$

f. If $1 < Z \le Z_f$, then compute the sample variance and standard deviation at θ:[12, 15]

$$s_Z^2(\theta) \leftarrow \frac{1}{(Z-1)}\left\{\sum_{Z=1}^{Z} n_Z^2(\theta) - \frac{1}{Z}\left[\sum_{Z=1}^{Z} n_Z(\theta)\right]^2\right\} = \frac{1}{(Z-1)}\left\{\Phi_Z(\theta) - \frac{1}{Z}\Psi_Z(\theta)\right\}$$

$$s_Z(\theta) \leftarrow [s_Z^2(\theta)]^{1/2}$$

Step 7. Advance θ by a suitably small $\Delta\theta$ as $\theta \leftarrow (\theta + \Delta\theta)$. If ($\theta \le t_f$), then return to Step 5; otherwise, go to Step 10.

Step 8. Determine the state of the system at the end of time interval $(t, t+\tau)$. At this juncture, a death event occurs, i.e., the population of bacteria decreases by one; thus,

$$n_Z(t) \leftarrow [n_Z(t-\tau)-1]$$

$$n_Z(\theta) \leftarrow n_Z(t)$$

Step 9. Repeat Steps 3 through 8 until t_f is reached.

Step 10. Update simulation counter as $Z \leftarrow (Z + 1)$.

Step 11. Repeat Steps 2 through 10 until Z_f is reached.

Appendix G. Additional Figures

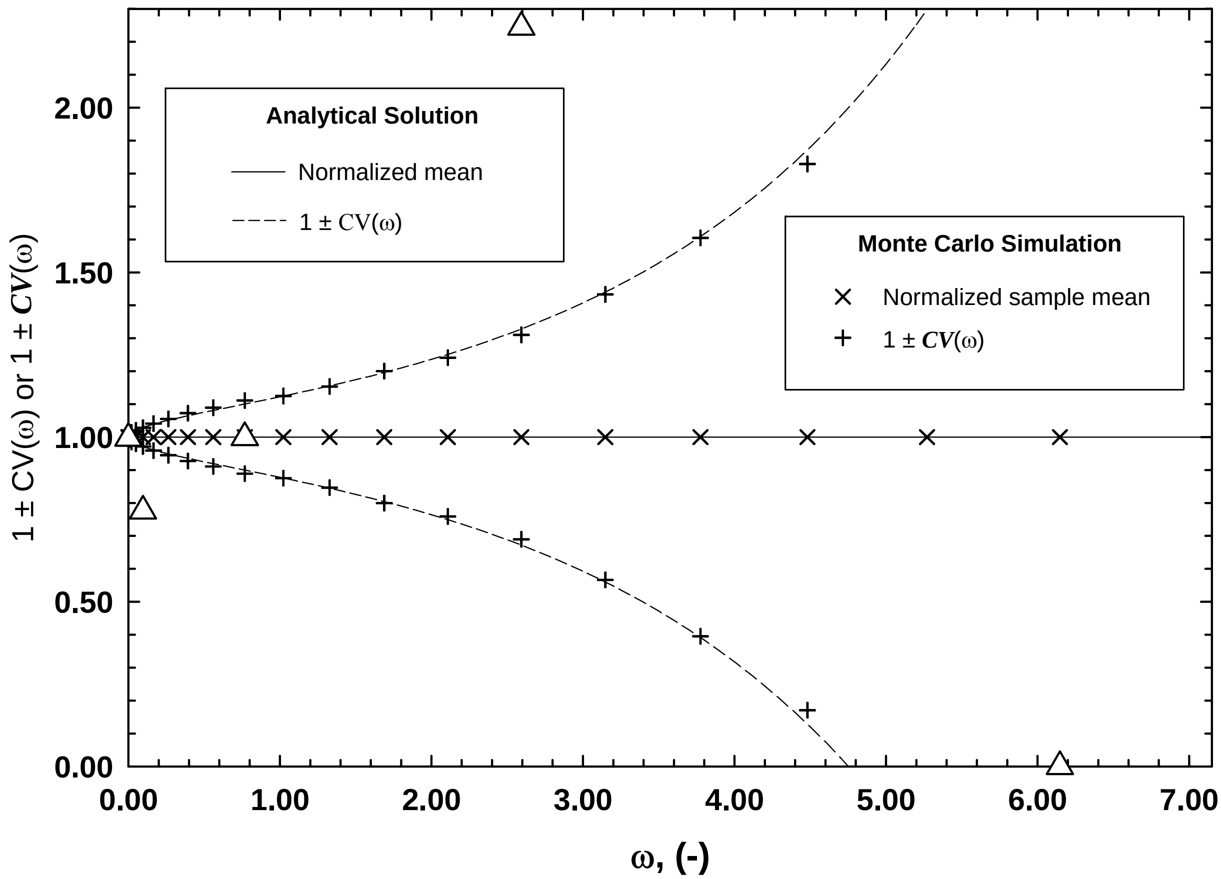

Figure G.1. Temporal evolution of the coefficient of variation, CV(ω), and the sample coefficient of variation, ***CV***(ω), of random variable N(ω) in the termination period of photoelectrochemical disinfection of *E. coli*[16] with n_0 = 115 cells per milliliter. Symbol (△) represents the normalized experimental data, ν(ω).

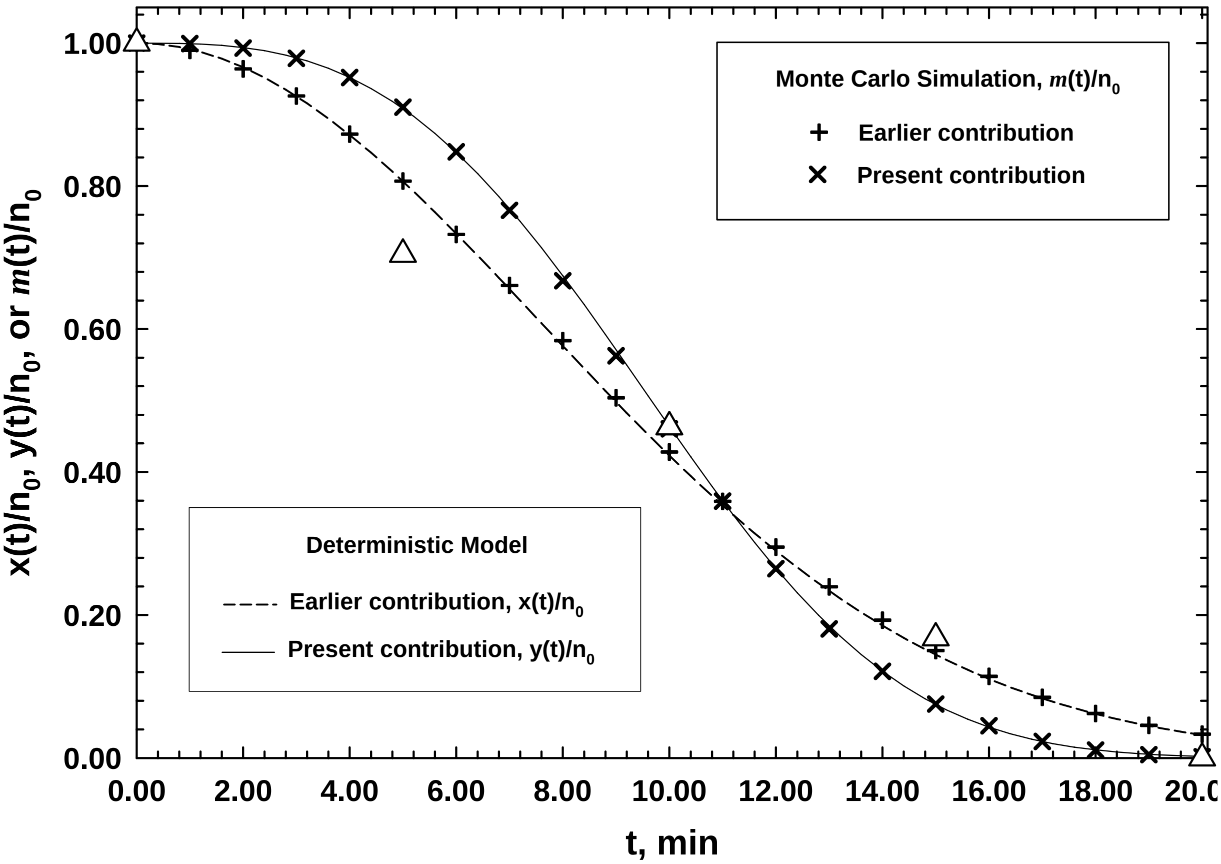

Figure G.2. Comparison of the Monte Carlo estimates for the dimensionless sample mean, $\boldsymbol{m}(t)/n_0$, based on our present and earlier[3] models in the termination period of photoelectrochemical disinfection of *E. coli*[16] with n_0 = 115 cells per milliliter. Symbol (△) represents the dimensionless experimental data, η(ω).

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