



Stochastic simulation for death probability of bacterial population considering variability in individual cell inactivation time and initial number of cells



Kento Koyama, Hiroki Abe, Shuso Kawamura, Shigenobu Koseki*

Graduate School of Agricultural Science, Hokkaido University, Kita-9, Nishi-9, Kita-ku, Sapporo 060-8589, Japan

ARTICLE INFO

Keywords:

Monte-Carlo simulation
Contour line
Poisson distribution
Weibull distribution

ABSTRACT

Decimal reduction time (D -value) based on the first-order survival kinetics model is not sufficient for reliable estimation of the bacterial survivors of inactivation treatment because the model does not consider inactivation curvature. However, even though doubt exists in the calculation of D -value, it is still widely used for risk assessment and sterilisation time estimation. This paper proposes an approach for estimating the time-to-inactivation and death probability of bacterial population that considers individual cell heterogeneity and initial number of cells via computer simulation. In the proposed approach, Weibull and Poisson distributions are respectively used to provide individual cell inactivation time variability and initial number of cells variability. Our simulation results show that the time-to-inactivation significantly depends on kinetics curvature and initial number of cells. For example, with increases in the initial number of cells, the respective variance of the time-to-inactivation of log-linear, concave downward curve, and concave upward curve remains constant, decreases, and increases, respectively. The death probability contour plot was successfully generated via our computer simulation approach without using D -value estimation. Further, the death probability calculated using our stochastic approach was virtually the same as that obtained using inactivation kinetics. We validated the simulation by using literature data for acid inactivation of *Salmonella* population. The results of this study indicate that inactivation curvature can replace D -value extrapolation to estimate the death probability of bacterial population. Further, our computer simulation facilitates realistic estimation of the time-to-inactivation of bacterial population. The R code used for the above stochastic calculation is outlined.

1. Introduction

The changes in average number of bacterial survivors are typically described using inactivation kinetics. The traditional model is log-linear inactivation kinetics and microbial inactivation is considered as a process that follows first-order-kinetics in this theory (Peleg and Cole, 1998). Decimal reduction time (D -value) is defined from log-linear inactivation. Further, inactivation curves with upward or downward concavity has been developed, because many inactivation behaviour show curvatures (Peleg and Cole, 1998; Xiong et al., 1999). Although microbial inactivation does not always follow the log-linear model, D -value is still widely used for risk assessment and sterilisation time estimation (Brown, 2002; Peleg and Normand, 2004). However, the accuracy of D -value calculation is in doubt (Koseki et al., 2009; Koyama et al., 2017a; Peleg, 2006). Because of the curvature of inactivation kinetics, overestimation or underestimation of bacterial survivors can

occur based on D -value (Peleg, 2006). In addition, the death probability of bacterial population is not estimated precisely because of extrapolation of D -value. In fact, the worst-case scenario is generally used to estimate bacterial survival probability in order to avoid overly optimistic risk assessments (Couvert et al., 2010; FAO/WHO, 2008; Membré et al., 2006; Zwietering et al., 1996). As a result, assessment results tend to overestimate bacterial survival in worst-case scenarios. Recently, Aspidou and Koutsoumanis (2015) indicated that the time required for 1-log reduction should not be a single point, but rather a probability distribution, as the population decrease below 100 cells. The death probability of bacteria population has also been estimated using probability distribution (Koyama et al., 2017a). Thus, a probabilistic approach describing variability in bacterial behaviour is a realistic alternative to D -value based estimation.

Variability in bacterial behaviour is studied because risk assessment required for the probability model (Brown, 2002; Codex Alimentarius

* Corresponding author.

E-mail address: koseki@bpe.agr.hokudai.ac.jp (S. Koseki).

<https://doi.org/10.1016/j.ijfoodmicro.2018.10.009>

Received 31 January 2018; Received in revised form 30 August 2018; Accepted 5 October 2018

Available online 08 October 2018

0168-1605/ © 2018 Elsevier B.V. All rights reserved.

Commission, 2009; FAO/WHO, 2008; Ross and McMeekin, 2003; Voysey and Brown, 2000). One important source of variability is individual cell heterogeneity, which is reflected in the population inactivation curve (Koutsoumanis and Aspridou, 2016). Individual cell heterogeneity is shown as individual cell inactivation time in inactivation kinetics (Koutsoumanis and Aspridou, 2016). Thus, it is possible to describe individual cell heterogeneity as a probability distribution. Variability in initial number of cells has been described as a Poisson distribution (Aguirre et al., 2009; Koyama et al., 2017b; Nauta, 2000). Further, Poisson distribution is used to describe randomly distributed initial cells in ideal conditions (Standaert et al., 2005). One other variability source is strain (van Asselt and Zwietering, 2006). These variabilities have all been described as probability distributions. However, these variabilities have not been integrated into inactivation kinetics to overcome the conventional death probability calculation based on D -value.

Before introducing the probability model, mathematical assumptions such as first-order-kinetic assumption for the log-linear model first have to be considered and defined. The log-linear model and D -value were developed (Peleg, 2006) and used for death probability calculation via mathematical calculation based on the concept of first-order-kinetic assumption. In the case of the probability model, the probability distribution underlying the kinetic model has to be considered. Individual cell heterogeneity is described from kinetic curvature (Koutsoumanis and Aspridou, 2016). Initial cell number is assumed under statistical aspect (Standaert et al., 2005). Defining variability as a probability distribution from a mathematical viewpoint is a first step toward probability modelling. Subsequently, bacterial inactivation should be studied based on this definition for comprehensive understanding of the process.

The objective of this study was to illustrate the time-to-inactivation and death probability of bacterial population via computer simulation considering the variability in individual cell inactivation time and initial cell number. Further, the death probability of the bacterial population was simulated with various initial cells and compared with the results calculated using inactivation kinetics. The proposed approach enables estimation of the risk of bacterial survival and selection of an appropriate bacterial population death probability without using conventional D -value extrapolation.

2. Material and methods

2.1. Mathematical-based assumption

In this study, stochastic population inactivation was simulated with variability in individual cell inactivation time and initial cell numbers. The following two assumptions were employed in the simulation. First, we assumed that bacterial inactivation kinetics follows the Weibull inactivation model with initial N_0 (i.e., $N_0 = 10^9$):

$$\log_{10} N(t) = -bt^n + \log_{10} N_0 \quad (1)$$

where t , $N(t)$, $\log_{10} N_0$, b , and n are the elapsed time, momentary number of survivors at time t , logarithm of number of initial cells, rate, and shape parameter of the Weibull distribution, respectively. The Weibull inactivation model is widely used for inactivation kinetics (Peleg, 2006; Peleg and Normand, 2004; van Boekel, 2002). Despite having developed a lot of survival models (Xiong et al., 1999), we picked up the Weibull model, because the Weibull model provides simply either concave upward or downward. In the case of bacterial inactivation, the individual inactivation time is reflected in the inactivation kinetics (Baranyi and Pin, 2001; Koutsoumanis and Aspridou, 2016; Peleg, 2006). According to the Weibull inactivation model, the inactivation rate of the population is changed as time elapses and inactivation of individual cell is considered to be an incidental countable event that is independent from other events. Thus, the individual cell inactivation time occurs randomly from the probability Weibull distribution.

Second, we assumed that the initial number of cells follows a Poisson distribution. If bacterial cells are randomly distributed in a liquid, then the number of bacteria in any portion of that liquid follows a Poisson distribution (El-Shaarawi et al., 1981; Standaert et al., 2005). Because when there is only a small amount of cells in liquid, the cells follow a Poisson distribution (Koyama et al., 2016), it is also conceivable that a large amount of cells also follows a Poisson distribution due to the reproductive property of the Poisson distribution. With the two assumptions outlined above, we simulated bacterial inactivation with variabilities in individual cell inactivation time and initial cell number. Third, we assumed that there is no recovery from injury cells and cells are either alive or death after the lethal treatment.

2.2. Procedure for computer simulation of bacterial inactivation

In our simulation, we referred to the methods used by Aspridou and Koutsoumanis (2015), who simulated bacterial inactivation using variability in individual cell inactivation time as individual cell heterogeneity. However, we added variability in initial cell numbers to our computer simulation, which differentiates it from their simulation. First, we determined the mean value of the initial number of cells N_0 ($\{N_0 \in \mathbb{R} \mid N_0 > 0\}$). The initial number of cells in the simulation was generated from a Poisson distribution as follows:

$$N'_0 \sim \text{Poisson}(N_0) \quad (2)$$

where N'_0 is the initial number of cells generated from the Poisson distribution with parameter N_0 . Next, we estimated the individual cell inactivation time for the N'_0 cells. Using inverse transform sampling from the cumulative Weibull distribution with rate and shape parameters, we estimated the individual cell inactivation time t_i of the i th cell as follows:

$$t_i \sim \text{Weibull}(b, n), i = 1, 2, 3 \dots N'_0 \quad (3)$$

For example, when the initial number of cells $N'_0 = 1000$, random sampling is generated 1000 times for individual cell inactivation time t_i of the i th cell. Then, we determined whether the i th cell survives or dies over time as follows:

$$\begin{aligned} t < t_i & S_i(t) = 1 \quad (\text{survival}) \\ t \geq t_i & S_i(t) = 0 \quad (\text{death}) \end{aligned} \quad (4)$$

where $S_i(t)$ is survival or death of the i th cell. Thus, the number of survivors $N(t)$ at time t is described as follows:

$$N(t) = \sum_{i=1}^{N'_0} S_i(t) \quad (5)$$

Eq. (5) describes one simulated survival curve. To replicate the above the simulation, stochastic bacterial inactivation was conducted via Monte Carlo simulation. In this study, we changed replication used in the simulation according to the purpose of the estimation. The R code used for the above stochastic calculation is outlined at R code viewer (Appendix A).

2.3. Trend of time-to-inactivation of bacterial population

To visualise the stochastic inactivation processes and time-to-inactivation, we simulated bacterial inactivation with different parameters of Weibull distribution and initial number of cells. Various parameters such as inactivation rate, and type of inactivation curve and number of initial cells were examined in the bacterial inactivation simulation (Table 1). In one condition, 100 replicates of bacterial inactivation were simulated. In each simulation, the maximum time of t_i became a random variable of the time-to-inactivation of the bacterial population. The time-to-inactivation of the bacterial population was illustrated as a histogram. Furthermore, we calculated the variance of the time-to-inactivation of the bacterial population with the initial

Download English Version:

<https://daneshyari.com/en/article/11263184>

Download Persian Version:

<https://daneshyari.com/article/11263184>

[Daneshyari.com](https://daneshyari.com)