Food Microbiology, 1999, **16**, 269–279 Article No. fmic.1998.0243
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ORIGINAL ARTICLE

Comparison of the Baranyi model with the modified Gompertz equation for modelling thermal inactivation of *Listeria monocytogenes* Scott A

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The Baranyi model was used to fit the four commonly observed survival curves: linear curves, those with a lag phase, those with a tailing phase and sigmoidal curves. It was validated by using published experimental data for thermal inactivation of Listeria monocytogenes *Scott A heated in infant formula and compared with the modified Gompertz equation. For the prediction performance, the Baranyi model was better and more robust than the modified Gompertz equation.*

Introduction

Thermal inactivation of micro-organisms has commonly been modelled using the first order kinetics. However, deviations from the first order kinetics are often observed (Cerf 1977, Kamau et al. 1990, Bhaduri et al. 1991, Linton et al. 1995, 1996, Adams and Moss 1997). Sometimes these deviations can be rationalised on the basis of some special property of the organism (Adams and Moss 1997). For example, the often observed lag and tailing regions in survival curves may reflect the presence of clumps of micro-organisms or a subpopulation of more heat-resistant micro-organisms. These deviations tend to be more common in the study of thermal death of vegetative organisms, which may reflect inadequacy of the logarithmic death concept (Adams and Moss 1997).

To model such nonlinear survival curves for vegetative organisms, several approaches have been proposed (Table 1). In earlier studies, various logistic equations were used. Cerf (1977) proposed a two-parallel-reactions model for describing biphasic curves. Kamau et al. (1990) applied three different forms of logistic equation to fit various shaped survival curves for *Listeria monocytogenes* heated in lactoperoxidase system. Whiting and Buchanan (1992) developed a logistic equation for describing the kinetics when there were significant shoulder and tailing in survival curves. This model was applied to non-thermal inactivation of *L. monocytogenes* (Buchanan et al. 1994, Buchanan and Golden 1995) and of *Staphylococcus aureus* (Whiting et al. 1996). Assuming a distribution of heat sensitivity within the population of heated cells, Cole et al. (1993) have also developed a vitalistic model that has been applied

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Received: 27 March 1998

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0740-0020/99/030269+11 $30·00/0

Table 1. Models for survival curves

Model	Mathematical Formula	Reference
First-order kinetics	$N = N_0 e^{-kt}$ or $\log \frac{N}{N_0} = -\frac{t}{D}$	
Cerf	$\frac{N}{N_0} = F_1 e^{-k_1 t} + (1 - F_1) e^{-k_2 t}$	Cerf (1977)
Kamau	For linear survival curves $\frac{N}{N_0} = \frac{2}{1 + e^{\beta t}}$ For survival curves with a lag phase $\log \frac{N}{N_0} = \log(1 + e^{-\beta t_{1/2}} - \log(1 + e^{-\beta t_{1/2}})$ For biphasic survival curves $\log \frac{N}{N_0} = \log\left(\frac{2F_1}{1 + e^{\beta_1 t}} + \frac{2(1 - F_1)}{1 + e^{\beta_2 t}}\right)$	Kamau et al. (1990)
Whiting and Buchanan	$\log \frac{N}{N_0} = \log\left(\frac{F_1(1 + e^{-\beta_1 t_L})}{1 + e^{\beta_1 (t - t_L)}} + \frac{(1 - F_1)(1 + e^{-\beta_2 t_L})}{1 + e^{\beta_2 (t - t_L)}}\right)$	Whiting and Buchanan (1992)
Cole	$\log N = \alpha + \frac{\omega - \alpha}{1 + e^{4\sigma(\tau - \log t)/(\omega - \sigma)}}$	Cole et al. (1993)
Gompertz	Modified Gompertz equation $\log N = A - Ce^{-e^{-B(t - M)}}$ or $\log \frac{N}{N_0} = Ce^{-e^{BM}} - Ce^{-e^{-B(t-M)}}$	Bhaduri et al. (1991); Linton et al. (1995, 1996)
Membre	$\log N = (1 + \log N_0) - e^{kt}$	Membre et al. (1997)

to thermal destruction kinetics of micro-organisms like *L. monocytogenes* (Cole et al. 1993, Stephens et al. 1994), *Salmonella typhimurium* (Ellison et al. 1994) or *Yersinia enterocolitica* (Little et al. 1994). Recently, Membre et al. (1997) proposed a logistic function to model the non-thermal inactivation of *S. typhimurium* in reduced calorie mayonnaise.

Nonlinear survival curves have also been modelled using the modified Gompertz equation. The Gompertz equation and its modified forms were used primarily in modelling the asymmetrical sigmoidal shape of microbial growth curves (McMeekin et al. 1993, Linton et al. 1995). Bhaduri et al. (1991) first demonstrated that the modified Gompertz equation can model the nonlinear survival curves for *L. monocytogenes* heated in liver sausage slurry, and that it is likely to provide a more accurate estimate of a micro-organism's thermal resistance than a first order kinetic model when dealing with sigmoidal survival curves. More recently, Linton et al. (1995, 1996) used the modified Gompertz equation to fit nonlinear survival curves for *L. monocytogenes* Scott A heated in infant formula and found that it was effective in modelling sigmoidal survival curves. However, the parameters of the modified Gompertz equation have not been directly linked with microbial death kinetics when using the logarithmic number of cells.

The purposes of this study are to use the Baranyi model for describing nonlinear survival curves of micro-organisms and to compare it with the modified Gompertz equation using established inactivation data for *L. monocytogenes* Scott A.

Materials and Methods

The Baranyi model

The Baranyi model has been originally developed for growth curves (Baranyi et al. 1993, Baranyi and Roberts 1994) and its goodness-of-fit is better than the modified Gompertz equation (Buchanan et al. 1997). To model sigmoidal survival curves such as curve SC4 in Fig. 1, it can be expressed as:

$$\begin{cases} \dfrac{\mathrm{d}N}{\mathrm{d}t} = -k_{\max}\alpha(t)N\beta(t) & (N > 0; t \geq 0) \\ N(0) = N_0 & (N_0 > 0; t = 0) \end{cases} \quad (1)$$

where N and N_0 are the number of micro-organisms present at time t and zero, respectively; $k_{\max}$ is the maximum relative death rate; $\alpha(t)$ is the shoulder adjustment function; $\beta(t)$ is the tailing adjustment function; minus sign means the inactivation of micro-organisms.

Although the change of the relative death rate $(1/N)(\mathrm{d}N/\mathrm{d}t)$ during the transitions among the lag, linear (namely log linear) and tailing phases is great, it is small and practically negligible during the linear phase. Therefore, the maximum relative death rate $k_{\max}$ can be thought of as the death rate constant for the linear phase of a survival curve. The shoulder adjustment function $\alpha(t)$ can take the following forms:

$$\alpha(t) = 1 - e^{-rt}$$

$$\alpha(t) = 1 - \frac{r^n}{r^n + t^n}$$

$$\alpha(t) = \frac{q_0}{q_0 + e^{-rt}}$$

$$\alpha(t) = \frac{1 - e^{-rt}}{1 + e^{-rt}} \quad (2)$$

where e is the Naperian base; r, q_0 and n are parameters. In this study it has been found that $\alpha(t) = 1 - [r^n/(r^n + t^n)]$ is the most suitable empirical function to describe the lag phase for the survival curves. The lag parameter r is the time required for the relative death rate to reach half of the maximum relative death rate $k_{\max}$. The parameter n is the curvatural parameter (Baranyi et al. 1993).

The original function $\beta(t)$ in the Baranyi model is designed for growth curves and not suitable for survival curves. In this study it has been found that the following empirical function (Eqn (3)) can be used as the tailing adjustment function for describing the tailing phase in survival curves such as curve SC3 or SC4 in Fig. 1.

$$\beta(t) = 1 - \frac{N_{\min}}{N} \quad (3)$$

where $N_{\min}$ is the minimum cell concentration remained in the tailing phase. When $N_{\min} \equiv 0$, it means that there is no tailing phase, while there is a tailing phase in a survival curve when $N_{\min} \neq 0$. Although the tailing function $\beta(t)$ varies greatly during the transition from the linear phase to the tailing phase, it is approximately equal to 1·0 during the lag and linear phases because $N_{\min}$ is usually much smaller than N.

After an integration, the solution of Eqn (1) can be given by:

$$N = N_{\min} + (N_0 - N_{\min})e^{-k_{\max}(t - B(t))} \quad (4)$$

where $B(t) = \int_0^t [r^n/(r^n + s^n)]\mathrm{d}s$ is the lag time function. In this study it was found that the shoulder adjustment function of $n = 3$ produces a satisfactory result in characterising

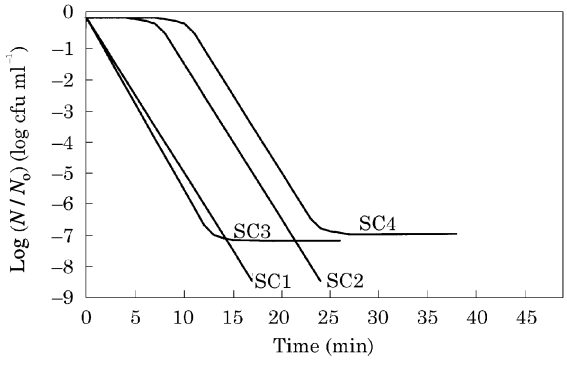

Figure 1. Graphic representations of four different shapes of survival curves.

the transition from the lag phase to the linear phase. When $n = 3$, $B(t)$ can be expressed by:

$$B(t) = \frac{r}{3}\left(\frac{1}{2}\ln\frac{(r+t)^2}{r^2 - rt + t^2} + \sqrt{3}\arctan\frac{2t-r}{r\sqrt{3}} + \sqrt{3}\arctan\frac{1}{\sqrt{3}}\right). \quad (5)$$

In terms of the base 10 logarithm, Eqn (4) can be rewritten as:

$$\log\frac{N}{N_0} = \log(q_B + (1-q_B)e^{-k_{\max}(t-B(t))}) \quad (6)$$

where $q_B = (N_{\min}/N_0)$ is the tailing ratio. Like $N_{\min}$, q_B can be used to indicate whether or not a tailing region exists. The benefit using the tailing ratio q_B is to avoid the direct use of the initial number N_0. In the case of multiple experiments, the initial numbers are usually different (Linton et al. 1995, 1996) and Eqn (4) can not be applied directly, although Eqn (6) can.

Although Eqn (4) or Eqn (6) are derived from the survival curves of curve SC4 (Fig. 1), it can be used to model the survival curves of curves SC1, SC2 and SC3 in Fig. 1. For example, if there is no tailing in the survival curves (namely $q_B \equiv 0$), Eqn (6) becomes:

$$\log\frac{N}{N_0} = -\frac{t - B(t)}{D_{\min}} \quad (7)$$

where $D_{\min} = 2{\cdot}303/k_{\max}$. Because $k_{\max}$ can be treated approximately as the death rate constant in the linear phase, the corresponding decimal reduction time is called the minimum decimal reduction time $D_{\min}$, which is the minimum time required for a one-log-cycle reduction of the micro-organism population at a reference temperature. When the lag parameter r in $B(t) = 0$, Eqn (7) becomes the well-known first order kinetic model (Eqn (8)) which can describe survival curves of curve SC1 (Fig. 1).

$$\log\frac{N}{N_0} = -\frac{t}{D} \quad (8)$$

where $D = 2{\cdot}303/k$ is the decimal reduction time or D-value; k is the death rate constant.

The modified Gompertz equation

The modified Gompertz equation was also developed for growth curves (Gibson et al. 1988). When it models sigmoidal survival curves (curve SC4 in Fig. 1), it can be expressed empirically by Eqn (9) (Bhaduri et al. 1991):

$$\log N = A - Ce^{-e^{-B(t-M)}} (t \geq 0) \quad (9)$$

where A is the value of the upper asymptote; B is the relative death rate at M; C is the difference in value of the upper and lower asymptote; M is the time at which the absolute death rate is maximal; minus sign before C means the inactivation of micro-organisms. The following kinetic parameters can be derived from Eqn (9) (McMeekin et al. 1993):

maximum (exponential) death rate $\mu_{\max}$

$$\mu_{\max} = \frac{BC}{e} \quad (10a)$$

lag phase duration t_{lag}

$$t_{\text{lag}} = M - \frac{1}{B} + \frac{\log N_0 - A}{\frac{BC}{e}} \quad (10b)$$

minimum cell concentration (the value of the lower asymptote) $N_{\min}$

$$\log N_{\min} = A - C = \log N_0 + Ce^{-e^{BM}} - C \quad (10c)$$

tailing ratio q_G

$$\log q_G = \log\frac{N_{\min}}{N_0} = Ce^{-e^{BM}} - C. \quad (10d)$$

To avoid the direct use of different initial numbers (N_0) in the case of multiple experiments, Eqn (9) can be rearranged to Eqn (11) (Linton et al. 1995, 1996) as

$$\log\frac{N}{N_0} = Ce^{-e^{BM}} - Ce^{-e^{-B(t-M)}}. \quad (11)$$

Comparing the modified Gompertz equation with the Baranyi model, it is interesting to find that $\mu_{\max}, t_{\text{lag}}$ and q_B are equivalent to $k_{\max}, r$ and q_G respectively.

Two-step procedure of modelling survival curves

To model survival curves, the widely-used two-steps of analysis are individual model analysis and full model analysis. Individual model analysis is defined as a process in which each

individual survival curve is fitted by the primary model such as the modified Gompertz equation (Eqn (11)) and the Baranyi model (Eqn (6)). The purposes of this analysis are to estimate the model parameters (such as $r, k_{\max}$ and q_B in Eqn (6), B, C and M in Eqn (11)) and to test the fitness of a model to the individual survival curves.

Full model analysis is defined as a process in which the model parameters from the individual model analysis are related to the environmental factors (such as temperature, pH, NaCl) using the secondary model, and then each individual survival curve is predicted by both the primary model and the predicted model parameters from the secondary model. The purpose of this analysis is to estimate the predicted model parameters by the secondary model and to test the prediction performance of a model. In practice it is more valuable than the individual model analysis.

In this study, the Response Surface Method (Eqn (12)) (Buchanan and Philips 1990) was used as the secondary model to relate the model parameters to the environmental factors.

$$y = a_0 + \sum a_i\ x_i + \sum_{i \neq j} a_{ij}\ x_i\ x_j + \sum a'_i\ x_i^2 \qquad (12)$$

where y is a model parameter (e.g. $r, k_{\max}$ or q_B in Eqn (6); B, C or M in Eqn (11)); x_i and x_j are the ith and jth environmental factors (temperature, pH or NaCl concentration), respectively; $a_0\ a_i\ a_{ij}\ a'_i$ are coefficients estimated from the experimental data.

In order to stabilize the variance of the data, the natural logarithmic (ln) transformation of model parameters was used (Gibson et al. 1988, Buchanan and Philips 1990). Because the tailing ratio q_B equals zero in some cases, the ln transformation is no longer valid. After several transformations were evaluated it was found that the transformation $\sqrt[4]{q_B}$ was the most effective to reduce the variance.

Experimental data and data analysis

The tested organism was *L. monocytogenes* Scott A (Linton et al. 1996). The experimental data consist of 59 different treatments, of which 27 and 32 treatments were used as model generation data and model validation data respectively (Linton et al. 1996).

To compare the performance of different models the correlation coefficient (R^2) and root mean square error (RMSE) between experimental data and those predicted using different models were applied. SPSS package (Release 6.1.2), MINITAB package (Release 11.11) and Microsoft Excel (version 5.0a) were employed in data analysis. For nonlinear regression, the estimation method of Sequential Quadratic Programming in SPSS package was used.

Results and Discussion

Individual model analysis

In individual model analysis it was found that both the Baranyi model (Eqn (6)) and the modified Gompertz equation (Eqn (11)) are effective in modelling curves with different shapes, including linear curves, curves with a shoulder or a tailing and sigmoidal curves, but neither of them consistently produces the best fit to all the survival curves. Overall, in terms of the RMSE and R^2 values listed in Table 2, the modified Gompertz equation fits better 2/3 of the total 27 survival curves from the model generation data, while the Baranyi model does better in 1/3 of the curves. However, it is also found that the Baranyi model produces better fit than the modified Gompertz equation when using the model validation data (see validation analysis below). By considering the set of model generation data as a whole, the performance of the modified Gompertz equation (RMSE = 0·1741, R^2 = 0·9918) is slightly better than the Baranyi model (RMSE = 0·1916, R^2 = 0·9903).

Although both models give similar fitting to the survival curves, there are significant differences between them. The first order kinetics model can be derived from the Baranyi model, but not from the modified Gompertz equation. The Baranyi model produces a practically straight line in the linear phase (Fig. 2(b)) but the modified Gompertz equation does not (Fig. 2(c)) because it does not assume a constant

Table 2. Results of individual model analysis and full model analysis using model generation data

Experiment No.	Temperature (°C)–pH–NaCl (%)	Individual model analysis						Full model analysis					
		Eqn (7)[a]		Eqn (6)[a]		Eqn (11)[b]		Eqn (7)		Eqn (6)		Eqn (11)	
		R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE
1	50-5-0	0·993	0·103	0·993	0·103	0·999	0·043	0·989	0·244	0·981	0·264	0·977	0·365
2	50-5-2	0·998	0·074	0·998	0·074	0·999	0·058	0·992	0·205	0·997	0·347	0·998	0·247
3	50-5-4	0·976	0·314	0·998	0·098	0·098	0·099	0·975	0·450	0·995	0·361	0·997	0·505
4	50-6-0	0·992	0·165	0·992	0·167	0·996	0·115	0·990	0·434	0·987	0·373	0·976	0·412
5	50-6-2	0·995	0·146	0·995	0·146	0·997	0·115	0·994	0·473	0·996	0·381	0·995	0·688
6	50-6-4	0·986	0·220	0·986	0·220	0·987	0·212	0·987	0·245	0·987	0·241	0·985	0·281
7	50-7-0	0·992	0·167	0·992	0·167	0·998	0·092	0·979	0·763	0·974	0·655	0·995	0·949
8	50-7-2	0·993	0·162	0·995	0·135	0·997	0·109	0·994	0·197	0·994	0·194	0·991	0·188
9	50-7-4	0·985	0·187	0·985	0·187	0·991	0·144	0·984	0·312	0·985	0·325	0·989	0·380
10	55-5-0	0·970	0·402	0·999	0·052	0·999	0·072	0·969	0·496	0·982	0·394	0·992	0·259
11	55-5-2	0·964	0·460	0·994	0·181	0·997	0·139	0·964	0·508	0·991	0·302	0·987	0·864
12	55-5-4	0·947	0·493	0·968	0·381	0·978	0·320	0·945	0·791	0·961	0·460	0·952	0·602
13	55-6-0	0·990	0·227	0·990	0·226	0·988	0·241	0·990	0·334	0·989	0·402	0·983	0·930
14	55-6-2	0·995	0·135	0·995	0·135	0·995	0·130	0·996	0·331	0·995	0·340	0·994	0·519
15	55-6-4	0·989	0·164	0·989	0·164	0·995	0·113	0·980	0·257	0·982	0·304	0·993	0·413
16	55-7-0	0·992	0·204	0·997	0·122	0·996	0·138	0·992	0·397	0·993	0·423	0·994	0·874
17	55-7-2	0·977	0·203	0·977	0·203	0·979	0·194	0·977	0·422	0·977	0·544	0·977	0·413
18	55-7-4	0·993	0·197	0·993	0·091	0·992	0·101	0·993	0·295	0·991	0·192	0·985	0·154
19	60-5-0	0·961	0·251	0·994	0·110	0·998	0·063	0·970	0·438	0·991	0·467	0·998	0·153
20	60-5-2	0·998	0·059	0·998	0·057	0·997	0·076	0·998	0·237	0·986	0·210	0·990	0·224
21	60-5-4	0·975	0·257	0·998	0·064	0·998	0·064	0·975	0·566	0·990	0·193	0·994	0·517
22	60-6-0	0·996	0·115	0·996	0·115	0·993	0·143	0·994	0·302	0·950	0·416	0·992	0·301
23	60-6-2	0·988	0·210	0·988	0·210	0·989	0·205	0·982	0·403	0·983	0·343	0·986	0·362
24	60-6-4	0·897	0·649	0·895	0·619	0·895	0·619	0·870	0·696	0·877	0·715	0·845	0·858
25	60-7-0	0·991	0·165	0·993	0·141	0·991	0·167	0·995	0·175	0·992	0·158	0·990	0·213
26	60-7-2	0·992	0·133	0·997	0·079	0·998	0·075	0·991	0·398	0·992	0·299	0·990	0·530
27	60-7-4	0·993	0·140	0·994	0·140	0·997	0·104	0·991	0·459	0·989	0·831	0·992	0·586
Whole data		0·985	0·240	0·990	0·192	0·992	0·174	0·955	0·454	0·964	0·430	0·940	0·613

[a]The Baranyi model (Eqn (6) and Eqn (7). Eqn (6) becomes Eqn (7) when the tailing ratio q_B is set to be zero).
[b]The modified Gompertz equation (Eqn (11)).

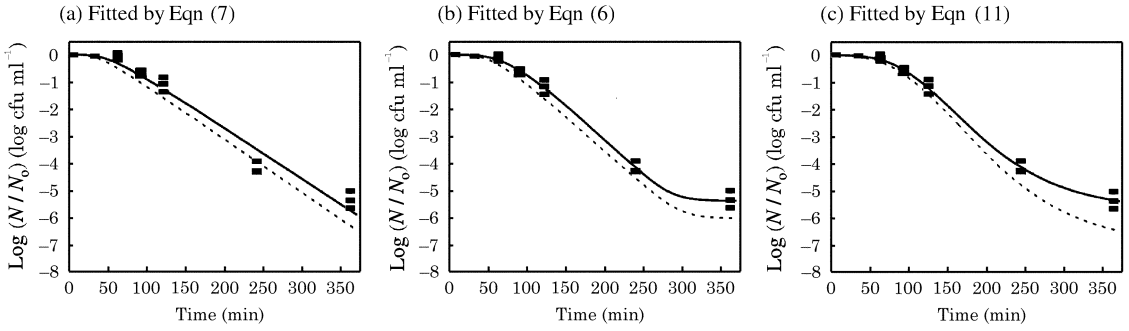

Figure 2. Survival curve fittings for *Listeria monocytogenes* Scott A following a treatment at temperature of 50°C, pH of 5 and NaCl of 4%: experimental data (▬), individual model fitting (——) and full model fitting (- - - - -). The Baranyi model (Eqn (6) (a) becomes Eqn (7) (b) when the tailing ratio q_B is set to zero and the modified Gompertz equation (Eqn (11)) (c).

death rate (Linton et al. 1995). The modified Gompertz equation always uses three parameters to fit the four commonly observed types of survival curves (curves SC1, SC2, SC3 and SC4 in Fig. 1), while the Baranyi model can use three or less number of parameters to fit the same types of the curves. For example, if all the survival curves investigated are ones with a shoulder or a tailing, the Baranyi model fits the curves by using two parameters $k_{\max}$ and r or q_B; if all the survival curves investigated are linear, the Baranyi model becomes the first order kinetic model (Eqn (8)) and fits the curves using one single parameter k. It is obviously unnecessary to use the modified Gompertz equation for fitting the linear curves and maybe the curves with a shoulder or a tailing.

It is found that the estimates of $t_{\text{lag}}, \mu_{\max}$ and q_G are similar to those of $r, k_{\max}$ and q_B (data not shown). For example, for the treatment of 50°C, pH 5 and 4% NaCl (Fig. 2), the estimates for Eqn (6) are $r = 75{\cdot}85$ min, $k_{\max} = 0{\cdot}0627$ (log cfu ml^{-1}) min^{-1}, $q_B = 4{\cdot}53 \times 10^{-6}$, and those for Eqn (11) are $t_{\text{lag}} = 79{\cdot}43$ min, $\mu_{\max} = 0{\cdot}0276$ (log cfu ml^{-1}) min^{-1} and $q_G = 6 \times 10^{-7}$ respectively. However, the differences are also observed. The estimated $k_{\max}$ and q_B values are greater than the $\mu_{\max}$ and q_G values for 98·31% and 66·10% of the 59 treatments (including both model generation and validation data) respectively and the estimated r values are smaller than the t_{lag} values for 86·44% of the 59 treatments. In the Baranyi model, 32·20% of the estimated q_B values are zero but none of the q_G values in the modified Gompertz equation are estimated to be zero.

The R^2 and RMSE values for Eqn (7) which is derived from Eqn (6) by setting q_B to be zero, are also listed in Tables 2 and 3. By comparing the difference in R^2 value between Eqn (6) and Eqn (7), the Baranyi model can indicate in some extent whether or not the tailing phase in a survival curve is significant, but the modified Gompertz equation cannot. In terms of the RMSE values Eqn (6) produces the same or better fitting than Eqn (7), which indicates that the better fitting survival curves have a tailing phase. However, the difference in R^2 values between Eqn (6) and Eqn (7) are usually very small, which suggests that the tailing phases may be not significant and may be caused by the variation of experimental data or model overfitting. An example is presented in Fig. 2.

Full model analysis

The R^2 and RMSE values for the two models (Eqn (6) and Eqn (11)) in the full model analysis are also listed in Table 2. It is found that the fitness of the models varies and neither of them can consistently produce the best fit to all the survival curves. Overall, the Baranyi model (Eqn (6)) fits better more than 2/3 of the total 27 survival curves from the model generation data and the modified Gompertz equation (Eqn (11)) does better in less than 1/3 of all the curves. By considering the set of the model generation data as a whole, the performance of the Baranyi model (RMSE = 0·430, $R^2 = 0{\cdot}964$) is significantly better than the modified Gompertz equation (RMSE = 0·613, $R^2 = 0{\cdot}940$).

Table 3. Results of the validation of the models using model validation data

Experiment No.	Temperature (°C)–pH–NaCl (%)	Individual model analysis						Full model analysis					
		Eqn (7)[a]		Eqn (6)[a]		Eqn (11)[b]		Eqn (7)		Eqn (6)		Eqn (11)	
		R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE
1	51-5·8-3·6	0·997	0·090	0·997	0·090	0·996	0·110	0·997	0·354	0·997	0·288	0·987	0·566
2	51-6·2-1·5	0·997	0·079	0·997	0·079	0·996	0·097	0·993	0·958	0·996	0·879	0·987	1·154
3	51-5·5-0·8	0·981	0·178	0·981	0·178	0·997	0·069	0·989	0·258	0·989	0·296	0·996	0·290
4	51-7·0-0·0	0·992	0·188	0·996	0·135	0·998	0·095	0·990	1·307	0·987	0·886	0·973	1·976
5	52-5·3-2·9	0·999	0·054	1·000	0·037	0·998	0·075	0·999	0·225	0·999	0·429	0·997	0·469
6	52-6·8-3·4	0·997	0·077	0·998	0·062	0·998	0·073	0·996	0·179	0·996	0·188	0·985	0·257
7	52-6·9-2·4	0·999	0·055	0·999	0·055	0·997	0·085	0·999	0·061	0·999	0·062	0·995	0·130
8	52-7·0-0·0	0·998	0·102	0·999	0·061	0·998	0·096	0·998	1·059	0·976	0·815	0·993	1·810
9	53-6·2-1·9	0·998	0·079	0·999	0·067	1·000	0·041	0·993	0·254	0·995	0·234	0·986	0·321
10	53-5·6-1·2	0·996	0·128	0·996	0·127	0·996	0·130	0·996	0·172	0·995	0·195	0·990	0·365
11	53-6·8-2·6	0·995	0·108	0·995	0·108	1·000	0·022	0·997	0·115	0·997	0·115	1·000	0·065
12	53-7·0-0·0	0·999	0·086	0·999	0·081	0·998	0·107	0·998	0·665	0·983	0·703	0·997	1·343
13	54-5·7-1·4	0·970	0·376	0·996	0·145	0·995	0·148	0·954	0·999	0·951	0·969	0·917	0·960
14	54-6·3-1·0	0·969	0·326	0·997	0·109	0·996	0·121	0·952	0·769	0·951	0·800	0·923	0·741
15	54-5·5-3·0	0·955	0·490	0·968	0·412	0·977	0·348	0·943	0·663	0·935	0·680	0·930	0·712
16	54-7·0-0·0	0·959	0·384	0·993	0·163	0·990	0·193	0·958	0·493	0·954	0·435	0·931	0·533
17	56-6·1-3·1	0·996	0·131	0·998	0·077	0·998	0·090	0·984	0·538	0·983	0·493	0·965	0·482
18	56-5·8-0·1	0·995	0·115	0·997	0·085	0·998	0·066	0·995	0·166	0·995	0·144	0·982	0·301
19	56-5·9-1·1	0·998	0·089	0·999	0·061	0·997	0·102	0·995	0·285	0·993	0·275	0·985	0·299
20	56-7·0-0·0	0·999	0·063	1·000	0·041	0·998	0·082	0·998	0·111	0·999	0·263	0·998	0·381
21	57-6·4-3·6	1·000	0·035	1·000	0·035	0·998	0·080	0·999	0·062	0·999	0·114	0·989	0·239
22	57-6·4-0·4	1·000	0·027	1·000	0·023	0·999	0·060	0·999	1·640	0·994	1·500	0·997	1·860
23	57-5·6-1·5	0·996	0·134	0·996	0·133	0·994	0·170	0·992	0·371	0·990	0·321	0·983	0·411
24	57-7·0-0·0	0·996	0·128	0·996	0·127	0·993	0·162	0·996	0·159	0·995	0·199	0·991	0·277
25	58-5·9-2·5	0·999	0·045	1·000	0·040	0·999	0·055	0·994	0·235	0·996	0·153	0·998	0·126
26	58-5·3-3·9	1·000	0·035	1·000	0·033	0·999	0·040	0·982	0·415	0·965	0·649	0·988	0·803
27	58-5·4-1·2	0·999	0·074	1·000	0·039	0·999	0·050	0·985	0·935	0·906	0·895	0·946	0·715
28	58-7·0-0·0	0·999	0·070	1·000	0·026	1·000	0·025	0·967	0·629	0·949	0·734	0·962	0·716
29	59-6·2-3·1	0·999	0·068	0·999	0·063	0·999	0·066	0·999	0·209	0·999	0·359	0·999	0·391
30	59-6·5-1·0	0·998	0·078	0·999	0·074	1·000	0·038	0·989	0·386	0·989	0·346	0·991	0·320
31	59-6·6-3·9	0·999	0·049	0·999	0·049	1·000	0·022	0·998	0·328	0·999	0·549	0·999	0·530
32	59-7·0-0·0	0·998	0·085	0·998	0·084	1·000	0·041	0·979	0·585	0·922	0·721	0·954	0·616
Whole data		0·993	0·166	0·997	0·116	0·997	0·112	0·918	0·629	0·928	0·595	0·900	0·818

[a]The Baranyi model (Eqn (6) and Eqn (7). Eqn (6) becomes Eqn (7) when the tailing ratio q_B is set to be zero).
[b]The modified Gompertz equation (Eqn (11)).

In addition, comparing the difference in RMSE or R^2 value between both the full-model analysis and the individual-model analysis, the Baranyi model seems more 'robust' than the modified Gompertz equation. The first reason for this is due to the structure of the models. Although both models can be used to fit sigmoidal survival curves, the structure of the Baranyi model is much more loose than that of the modified Gompertz equation. In the Baranyi model only one key parameter which cannot be equal to zero is the maximum relative death rate k_{max}, while the modified Gompertz equation has two key parameters B and C. The parameters r, k_{max} and q_B in the Baranyi model can describe the lag, linear and tailing phases in a direct way respectively, while the modified Gompertz equation describes these phases in a more complex way (Eqn (10)). For example, the Baranyi model uses k_{max} to describe the linear phase and gives a practical straight line, by contrast the modified Gompertz equation employs both B and C to describe the linear phase and gives a nonlinear curve. The second reason is that the Baranyi model and the modified Gompertz equation have different sensitivities to the changes of their parameters. By varying one parameter and holding other parameters constant for a model, a series of RMSE values can be calculated. This process is repeated until the RMSE values of all parameters involved are obtained. These RMSE values can then be used to compare the sensitivity of each parameter on the model. In terms of the same percentage variation, the parameters can be ordered from the most sensitive one to the least sensitive one. Among the three parameters of r, k_{max} and q_B in the Baranyi model, it is found that k_{max} is the most sensitive one followed by r and q_B, which matched the order of the R^2 values for the three parameters (Table 4). Although the R^2 value for the tailing ratio q_B is lower (0·697), q_B has a relatively small influence on the RMSE value because the Baranyi model is not very sensitive to it. By contrast, for the modified Gompertz equation the parameter C is the most sensitive one followed by M and B is the least sensitive one. A small change in the values of parameters C and M results in a large variation in RMSE value. The big RMSE value and small R^2 value for the modified Gompertz equation in the full model analysis may be caused in part by the parameter C due to its small R^2 value (0·700) (Table 4).

Validation analysis

Model validation provides information which shows the performance of a model performances in practice. In this study the model validation data consists of 32 different treatments which are different from the model generation data but use the environmental factors that are within the region for the full model analysis. The validation results are listed in Table 3. From Table 3, it is interesting to note that the overall performance of the Baranyi model

Table 4. Estimates for the coefficients of the model parameters

Effect terms	Eqn (7)[a]		Eqn (6)[a]			Eqn (11)[b]		
	$\ln(k_{max})$	$\ln(r)$	$\ln(k_{max})$	$\ln(r)$	$q_B^{1/4}$	$\ln(B)$	$\ln(C)$	$\ln(M)$
Intercept	22·5478	36·1419	23·2592	33·3836	1·7302	5·6125	4·6709	0·3057
Temperature	−1·2611	−1·7567	−1·0394	−1·3189	−0·0486	0·0537	−0·7894	−0·2127
pH	0·8592	9·0769	−1·4070	5·7739	−0·1797	−7·1579	7·6188	6·9924
NaCl	−0·6303	−1·6457	−0·7706	−1·2601	0·0677	1·0274	−1·9435	−1·2194
Temperature^2	0·0150	0·0136	0·0136	0·0104	0·0006	0·0043	0·0061	−0·0019
pH^2	−0·0489	−0·5516	0·1777	−0·2432	0·0260	0·6080	−0·6045	−0·5178
NaCl^2	0·0112	−0·0562	0·0275	−0·0242	−0·0005	−0·0232	0·0797	0·0208
Temperature × pH	−0·0097	−0·0405	−0·0196	−0·0488	−0·0025	−0·0120	−0·0029	−0·0070
Temperature × NaCl	0·0087	0·0299	0·0126	0·0259	−0·0008	−0·0117	0·0264	0·0179
pH × NaCl	−0·0092	0·0655	−0·0315	0·0154	−0·0039	−0·0669	0·0216	0·0480
R^2	0·984	0·967	0·964	0·949	0·679	0·972	0·700	0·982

[a]The Baranyi model (Eqn (6) and Eqn (7). Eqn (6) becomes Eqn (7) when the tailing ratio q_B is set to zero).
[b]The modified Gompertz equation (Eqn (11)).

(Eqn (6)) was better than that of the modified Gompertz equation (Eqn (11)) for both individual model analysis and full model analysis, i.e. the Baranyi model consistently produced better fit to more than 2/3 of the total 32 survival curves, while the modified Gompertz equation gave better fitness to less than 1/3 of the total curves validated. By considering the set of the model validation data as a whole, the RMSE and R^2 values for both the Baranyi model (RMSE = 0·116, R^2 = 0·997) and the modified Gompertz equation (RMSE = 0·112, R^2 = 0·997) were almost same for individual model analysis, but those for both the Baranyi model (RMSE = 0·595, R^2 = 0 ·928) and the modified Gompertz equation (RMSE = 0·818, R^2 = 0·900) were significantly different for full model analysis.

Conclusion

Although the Baranyi model is empirical when it is used for survival curves, it can model the four commonly observed survival curves: linear curves, curves with a lag phase, curves with a tailing phase and sigmoidal curves. For the prediction performance, the Baranyi model was better and more robust than the modified Gompertz equation.

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Appendix

Nomenclatures

N	number of micro-organisms, cfu ml^{-1}
N_0	initial number of microorganisms, cfu ml^{-1}
t	time, min
k	death rate constant, (log cfu ml^{-1}) min^{-1}
k_{max}	maximum relative death rate, (log cfu ml^{-1}) min^{-1}
D	decimal reduction time, min
D_{min}	minimum decimal reduction time, min
r	lag parameter, min
q_B	tailing ratio in the Baranyi model
n	curvatural parameter
N_{min}	minimum cell concentration, cfu ml^{-1}
A	lower asymptote, log cfu ml^{-1}
B	relative death rate at M, (log cfu ml^{-1}) min^{-1}
C	difference in value of the upper and lowerasymptote, log cfu ml^{-1}
M	time at which the absolute death rate is maximal, min
μ_{max}	maximum exponential death rate, (log cfu ml^{-1}) min^{-1}
t_{tag}	lag phase duration, min
q_G	tailing ratio
$\alpha(t)$	the adjustment function or shoulder adjustment function
$\beta(t)$	the tailing adjustment function
$B(t)$	the lag time function, min