# **RESEARCH ARTICLE**



# Development of a New Modelling Approach and Performance Evaluation of Meta-heuristic Optimization Algorithms for the Prediction of Kinetic Growth Parameters for *Pseudomonas spp.* in Fish

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# Abstract

The main aim of the current work was to build up a new mathematical modelling approach in predictive food microbiology field for the prediction of growth kinetics of microorganisms. For this purpose, the bacterial growth data of *Pseudomonas spp.* in whole fish (gilt-head seabream) subjected to isothermal and non-isothermal storage temperatures were collected from previously published growth curves. Maximum specific growth rate (1/h) and lag phase duration (h) were described as a function of storage temperature using the direct two-step, direct one-step and inverse dynamic modelling approaches based on various meta-heuristic optimization algorithms. The fitting capability of the modelling approaches and employed optimization algorithms was separately compared, and the one-step modelling approach for the direct methods and the Bayesian optimization method for the used algorithms provided the best goodness of fit results. These two were then further processed in validation step. The inverse dynamic modelling approach based on the Bayesian optimization algorithm yielded satisfactorily statistical indexes (1.02 > Bias factor > 1.09 and 1.07 > Accuracy factor > 1.13), which indicates it can be reliably used as an alternative way of describing the growth behaviour of *Pseudomonas spp.* in fish in a fast and efficient manner with minimum labour effort.

Keywords: Inverse dynamic modelling; meta-heuristic optimization; growth behaviour; predictive microbiology

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# INTRODUCTION

Predictive food microbiology is a relatively new field of theoretical research in food microbiology that describes the behaviour of microorganisms in food under variable environmental conditions by employing mathematical functions and statistical assessment.<sup>1</sup> Using models in predictive food microbiology, the conditions prevailing in food products that can decrease or delay adverse effects (e.g., spoilage) resulting from microbial load in food can be determined. Mathematical functions for prediction of microorganism behaviour are generally grouped into two categories, as primary and secondary models.<sup>2</sup> Microorganism behaviour under a static environmental condition is described by primary models as a function of time, while the secondary models are used to determine the effects of environmental factor and/ or food matrixes on model factors. Temperature is a critical external factor that plays a key role in microorganism behaviour in food products.

The two-step modelling method in which primary and secondary models are serially used is the most applied modelling approach in predictive microbiology. In this approach, the first step is to fit the bacterial growth data points with primary model by time. Afterward, microorganism kinetic parameters derived from the first step are defined as a function of external factors for example temperature, pH, and water activity with the secondary model.<sup>3</sup>

Even though this modelling approach usually provides acceptable predictions, there are some drawbacks. The major disadvantage is accumulated errors resulting from applying two times nonlinear regression process.<sup>4</sup> The onestep modelling approach is an alternative way of describing growth behaviour by overcoming the weaknesses of a two-step process. In this approach, all data points from different conditions were described by simultaneously employing primary and secondary models.<sup>5-7</sup> Furthermore, bacterial counts collected under dynamic conditions can be also described using the onestep modelling approach. This enables to define the kinetic parameters by performing only dynamic experiments that are more reflective of microbial behaviour rather than various static experiments which are frequently time consuming and labourintensive.8,9

Two-step and one-step modelling approaches are considered as direct fitting procedures by which primary and secondary models for static conditions either separately or simultaneously can be developed. Then predictive capabilities of these models can be assessed considering bacterial growth counts collected for changing environmental conditions. The inverse dynamic modelling approach is a new modelling method, an alternative to direct modelling methods. In this modelling process, the bacterial growth counts obtained from dynamic environmental conditions are directly used for model fitting by jumping of the first step of direct methods including static experiments which are often time-consuming and labour-intensive. Therefore, the inverse dynamic modelling approach can minimise experimental effort in a single step and be considered as a fast and inexpensive way of modelling.<sup>8</sup> So, the inverse dynamic modelling approach has a considerable potential as a simulation tool to predict growth behaviour of microorganisms and can pave a new alternative way for doing experimental plan in predictive food microbiology field.<sup>9</sup> In this regard, the advantages of the inverse dynamic modelling approach have been increasingly aroused interests in predictive food microbiology field, and some inspirational works have been published recently.9-11

The real-world optimization problems are becoming more complex and simple local optimization algorithms often remain insufficient. When there are no optimum solutions better than a local optimum, the latter can be regarded as the global solution (i.e., gold standard), which leads false predictions. Especially for nonlinear problems, there might be numerous local optimal solutions near the gold standard, and finding the global optimal point is a crucial step for the inverse dynamic modelling approach due to its nonlinearity and complexity. Therefore, for the implementation of the inverse dynamic modelling approach global optimization algorithms are necessary. Metaheuristic optimization algorithms are trying to find a global optimum point by avoiding multiple local solutions. Meta-heuristic optimization algorithms attract huge amount of interest due to their strong and obvious advantages over traditional optimization algorithms.<sup>12</sup>

The main goal of this study was to comprehensively assess the prediction capability of the inverse dynamic modelling approach based on various meta-heuristic optimization algorithms by considering growth kinetic parameters of *Pseudomonas spp.* in whole fish (gilt-head seabream) subjected to isothermal and nonisothermal storage temperatures.

# MATERIALS AND METHODS

The work took place in five separate steps: i) the growth data points of Pseudomonas spp. in fish subjected to isothermal and non-isothermal storage temperatures were collected, ii) for the direct modelling approach, two-step and one-step modelling methods based on the Baranyi and the Ratkowsky models were employed to find growth kinetics, iii) for the inverse modelling approach, the dynamic versions of the same models were applied. iv) the growth kinetics obtained from the direct and inverse modelling approaches were compared and v) maximum growth rate and lag phase duration values were used for model validation. The flow chart outlining the main steps followed in the current study is given in Fig. 1. Details of the stages in this work are described in the following subsections.

# Data collection

The bacterial growth data of *Pseudomonas* spp. under isothermal and non-isothermal storage conditions in fish were gathered from the growth curves in the relevant published study of KOUTSOUMANIS.13 The detail experimental procedure for acquiring Pseudomonas spp. growth data was explained in detail in the previous work. Briefly, fish samples were obtained from a fish industry in Athens and then immediately transferred to the laboratory. Storage temperatures of 0°C, 2°C, 5°C, 8°C, 10°C and 15°C were set and controlled in high-accuracy lowtemperature incubators for isothermal conditions. Experiments were conducted at suitable time intervals depending on their storage temperatures to effectively analyse the effect of temperature on bacterial growth. Traditional bacterial enumeration of Pseudomonas spp. was performed onto cetrimide fucidin cephaloridine (CFC) agar using the spread plate method. Incubators used and supplier information for CFC agar are referred in the original work of KOUTSOUMANIS.<sup>13</sup> Minimum three replicates were performed for each of the growth data points. In the present study, *Pseudomonas spp.* growth data were gathered from the growth curves which were given in the work of KOUTSOUMANIS,<sup>13</sup> with GetData Graph Digitizer 2.26 software (Digital River, Cologne, Germany).

# Modelling

# **Primary models**

The Baranyi model<sup>14</sup> was employed for fitting of the growth data points obtained from isothermal temperatures using the Eqs. (1) and (2), and from non-isothermal storage temperatures using the Eqs. (3) and (4):

$$y(t) = y_0 + \mu_{max}F(t) - ln\left(1 + \frac{e^{\mu_{max}F(t)} - 1}{e^{(y_{max} - y_0)}}\right)$$
....(1)

$$F(t) = t + \frac{1}{v} ln \left( e^{-vt} + e^{-\mu_{max}\lambda} - e^{(-vt - \mu_{max}\lambda)} \right)$$

....(2)

where t is the time (h), y(t) is the concentration of bacterial populations (ln CFU/g) at time t,  $y_o$  is the initial concentration of bacterial populations (ln CFU/g),  $y_{max}$  is the maximum population density (ln CFU/g),  $\mu_{max}$  is the maximum specific bacterial growth rate (1/h),  $\lambda$  is the duration of lag phase (h) and v is the rate of increase of limiting substrate, assumed to be equal to  $\mu_{max}$ .

$$\frac{dy(t)}{dt} = \mu_{max} \left[ \frac{1}{1 + exp(-Q(t))} \right] \{1 - exp(y(t) - y_{max})\} \dots (3)$$

$$\frac{dQ(t)}{dt} = \mu_{max} \qquad \dots (4)$$

where Q(t) is the natural logarithm of q(t), a dimensionless variable related to physiological state of the cells,  $y_{max}$  is the maximum population concentration (In CFU/g) obtained from the global model, and  $\mu_{max}$  (h<sup>-1</sup>) is a function of both temperature (T) and time (t). The initial conditions applied to solve Eqs. (3) and (4) were y(0) = y0 (i.e. the initial population concentration (In CFU/g)) and Q(0) = Inq0, respectively.

## Secondary Models

The Ratkowsky model<sup>15</sup> was applied for defining  $\mu_{max}$  as a function of temperature via the Eq. (5):

$$\sqrt{\mu_{max}} = b_1(T - T_0)$$
 .... (5)

where T is the storage temperature (°C),  $T_o$  is the theoretical lowest bacterial growth temperature (°C),  $\mu_{max}$  is the maximum specific bacterial growth rate (1/h), b1 is the regression coefficient.

Additionally,  $\lambda$  (lag phase duration) was defined as a function of  $\mu_{max}$  with respect to temperature using the Eq. (6)<sup>16</sup>:

where  $b_2$  is the regression coefficient,  $\mu_{max}(T)$  is a function of temperature, which leads  $\lambda$  to be defined as a function of storage temperature. Parameter estimation

In order to determine the kinetic parameters of *Pseudomonas spp.* in fish, NonLinearModel command which uses Levenberg Marquardt algorithm in the Matlab 8.3.0.532 (R2014a) software (MathWorks, Natick, Massachusetts, USA) was employed considering the direct two-step and one-step modelling approaches.

For the inverse dynamic modelling approach, each of the parameters  $(b_1, b_2)$  and  $T_0$  was estimated by minimising the difference between fitted and observed bacterial growth counts by using the Eq. (7):

$$obj = min \sum_{i=1}^{n} \{ f_{fit}(b_1, b_2, T_0) - f_{Obs} \}^2$$
...(7)

where *obj* is the objective function, minimization of difference between  $f_{fit}$  and  $f_{obs'}$ ,  $f_{fit}$  is the fitted values that satisfy the objective function,  $f_{obs}$  is the observed growth data and n is the number of experiments.

The optimization process was done with various algorithms (Simulated Annealing, Genetic, Bayesian, Particle Swarm and Quasi-Newton Algorithms) in the Global Optimization Toolbox in the Matlab software. Genetic is an evolutionary algorithm which uses the mutation to prevent from being stuck in local optimum while transferring knowledge to new epochs. Simulated Annealing and Particle Swarm optimization can be classified as global search metaheuristics. Quasi-Newton Algorithms can be defined as local search-based algorithms. Bayesian Optimization is a global optimizer which constructs a proxy function (such as Gaussian process approximation) that gives close results to the objective function with less computational cost. Therefore, different optimization algorithms are suggested to measure the efficiency of the inverse dynamic modelling approach.

Since the ordinary differential equations in the dynamic model of Baranyi has not an analytical solution,<sup>8</sup> numerical solution was obtained using the function ode23 existing in Matlab software, which is based on the Runge– Kutta method.

The 95% confidence intervals (CI) of the model parameters were calculated using the Eq. (8)<sup>17</sup>:

$$Cl = par \pm t_n \sqrt{S}$$
...(8)

where par is the parameter estimated by the fitting,  $t^n$  is calculated using the inverse of Student's t cumulative distribution function, S is a vector of the diagonal elements from the estimated covariance matrix of the coefficient estimates,  $(X^TX)_{-1}s^2$ , X is the Jacobian of the fitted values with respect to the parameters,  $X^T$  is the transpose of X,  $s^2$  is the mean squared error. **Comparison of the goodness of fit** 

The evaluation of prediction capability of the models was performed by considering the root

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mean square error (*RMSE*), adjusted coefficient of determination ( $R^2_{adj}$ ), corrected Akaike information criterion (*AICc*) and Bayesian information criterion (*BIC*) using Eqs. (9), (10), (11) and (12) respectively:

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(x_{obs} - x_{fit})^{2}}{n - s}}_{....(9)}$$

$$R_{\mathrm{adj}}^2 = 1 - \left(\frac{\mathrm{n}-1}{\mathrm{n}-\mathrm{s}}\right) \left(\frac{\mathrm{SSE}}{\mathrm{SST}}\right)$$

.... (10)

$$AIC_{\rm C} = (n)\ln\left(\frac{\rm SSE}{\rm n}\right) + 2(s+1) + \frac{2(s+1)(s+2)}{\rm n-s-2}$$
....(11)

$$BIC = n \ln\left(\frac{SSE}{n}\right) + s \ln(n)$$
 ...(12)

where  $x_{obs}$  is the experimental bacterial growth,  $x_{fit}$  is the fitted value, n is the number of experiments, s is the number of parameters of the model, *SSE* is the sum of squares of errors and *SST* is the total sum of squares.

#### Statistical analysis

Growth kinetic parameters obtained from the direct modelling approaches and inverse dynamic modelling approach were statistically evaluated by using *t-test* analysis via the Matlab software. Statistical differences between various modelling approaches were considered as significant once *p* was found less than 0.05.

# Validation of the models

The prediction capability of different modelling approaches and employed optimization algorithms was evaluated through maximum specific growth rate data of *Pseudomonas spp.* in fish gathered from the study of KOUTSOUMANIS.<sup>13</sup> The comparison was done considering each of the global models' factors corresponding to the bias  $(B_j)$  and accuracy  $(A_j)$  factors<sup>18</sup> given in Eqs. (13) and (14), respectively:

$$B_{\rm f} = 10^{\frac{\sum_{i=1}^{\rm n} \log{(x_{pred}/x_{obs})}}{\rm n}}$$

$$A_{\rm f} = 10^{\frac{\sum_{i=1}^{n} \left| \log \left( x_{pred} / x_{obs} \right) \right|}{n}}$$
...(14)

.... (13)

where xpred refers to predicted  $\mu_{max}$  (1/h) and  $\lambda$  (h),  $x_{obs}$  refers to experimental  $\mu_{max}$  (1/h) and  $\lambda$  (h), n refers to the number of experimental growth data.

# **RESULTS AND DISCUSSION**

The experimental Pseudomonas spp. counts collected from previously published curves for fish13 at the storage temperatures of 0°C, 2°C, 5°C, 8°C, 10°C and 15°C were used to implement the two-step and one-step modelling approaches based on the Baranyi model (Fig. 2). The initial bacterial counts of Pseudomonas spp. were on average  $3.3 \pm 0.4 \log \text{CFU} \cdot \text{g}^{-1}$  for all temperatures. Storage duration was directly related to storage temperature and ranged from 360 to 72 h (15 to 3 days) with an increase in storage temperature from 0 to 15°C. The Pseudomonas spp. counts could reach the level of 8.3  $\pm$  0.3 log CFU•g<sup>-1</sup> at the end of storage depending on the storage temperature. This demonstrated that the growth potential of Pseudomonas spp. in fish was not affected with the increasing storage temperature.

The goodness-of-fit of Baranyi model involved in direct two-step and one-step modelling approaches was evaluated by calculating their statistical indices (*RMSE*,  $R^2_{adf}$  *AICc* and *BIC*). The *RMSE* values obtained from direct two-step and direct one-step modelling approaches were 0.570 and 0.450, respectively, and  $R^2_{adj}$  values obtained from the direct two-step and direct one-step modelling were 0.910 and 0.940, respectively (Table 1). In addition, the *AICc* and *BIC* indices of direct two-step modelling approach were -78.2, -69.8, respectively, and the *AICc* and *BIC* indices of direct one-step modelling approach were -112.7 and -104.2, respectively (Table 1). These results presented that one-step modelling approach enhanced the fitting performance of the Baranyi model and could be more reliably used for estimation of *Pseudomonas spp.* in fish. Additionally, the lack of fitting capability of the direct two step modelling approach for 10 and 15°C was eliminated with the implementation of the direct one-step modelling approach (Fig. 2).

The degrees of freedom of the one-step modelling approach proposed in this study were 71 (the number of observations – the number of parameters in the global model), while the degrees of freedom of the traditional two-step modelling approach used by KOUTSOUMANIS,<sup>13</sup> were only 4 for the Ratkowsky model and were maximum 10 for the primary models at various temperatures ranging from 0 to 15°C. It is important to underline that especially the Ratkowsky model with a low degree of freedom might be regarded as giving results which are of low accuracy and uncertain. From this point of view, the one-step modelling approach followed has increased degrees of freedom, which decreases confidence intervals and uncertainty of the parameters compared to the traditionally used two-step modelling approach. Therefore, the one-step modelling approach significantly (p < 0.05) improved the prediction capability of the models for the quantitative description of *Pseudomonas spp.* in fish.

The experimental *Pseudomonas spp.* counts in fish at the dynamic storage temperatures ranging from 0 to 15°C were used for dynamic inverse modelling approach based on the Baranyi's model and various optimization algorithms (Fig. 3). *RMSE*,  $R^2_{adf}$ , *AICc* and *BIC* values of used optimization algorithms in inverse dynamic modelling approach were calculated. The *RMSE* and  $R^2_{adj}$  values were in range of 0.300 to 0.330 and 0.970 to 0.986, respectively (Table 1). Additionally, the *AICc* and *BIC* indices were calculated in range of -115.8 to -95.0 and -92.3 to -113.1, respectively. Although each of the optimization algorithms in





the inverse dynamic modelling approach yielded better fitting performances compared to direct modelling approaches (two-step and one-step modelling approaches), Bayesian optimization algorithm was the best in the inverse dynamic modelling approach (Table 1). and maximum growth rate of microorganism.  $T_o$  was equal to -12.46°C, and  $b_1$  was found to be 0.018°C-1.h0.5 in the inverse dynamic modelling approach. These results are in a good agreement with the work conducted by KOUTSOUMANIS,<sup>13</sup> who reported the values of T0 and b1 ranging from -12.96 to -10.64°C and 0.018 to 0.205°C<sup>-1</sup>.

 $T_o$  and  $b_1$  are the Ratkowsky parameters showing the relationship between temperature



Fig. 2. The observed and fitted Pseudomonas spp. in fish using direct a) two-step and b) one-step modelling approach.



**Fig. 3.** The observed and fitted *Pseudomonas spp.* in fish using inverse dynamic modelling approach for different temperature profiles. The dashed line shows the changing temperature during storage.

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| Fitting method   |                |                         | Model parameters     |                   | RMSE  | $R^2$ adj | AICc   | BIC    |
|------------------|----------------|-------------------------|----------------------|-------------------|-------|-----------|--------|--------|
|                  |                | Τ <sub>0</sub> (°C)     | b1                   | b2                |       |           |        |        |
| Direct approach  | Two-step       | -11.56 (-12.19, -10.93) | 0.019 (0.018, 0.021) | 1.78 (1.63, 1.83) | 0.570 | 0.910     | -78.2  | -69.8  |
|                  | One-step       | -8.58 (-9.04, -8.12)    | 0.024 (0.023, 0.025) | 1.41 (0.71, 2.10) | 0.450 | 0.940     | -112.7 | -104.2 |
| Inverse approach | Simulated      | -7.98 (-8.37, -7.58)    | 0.025 (0.024, 0.025) | 2.68 (2.52, 2.84) | 0.330 | 0.973     | -100.5 | -97.8  |
|                  | Annealing      |                         |                      |                   |       |           |        |        |
|                  | Genetic        | -6.32 (-6.52, -6.12)    | 0.027 (0.026, 0.028) | 2.33 (2.17, 2.48) | 0.307 | 0,977     | -107.7 | -105.0 |
|                  | Bayesian       | -12.46 (-13.17, -11.75) | 0.018 (0.018, 0.019) | 1.78 (1.64, 1.92) | 0.300 | 0.986     | -115.8 | -113.1 |
|                  | Particle Swarm | -5.59 (-6.00, -5.19)    | 0.029 (0.027, 0.030) | 2.84 (2.69, 3.00) | 0.350 | 0.970     | -95.0  | -92.3  |
|                  | Quasi-newton   | -13.45 (-14.62, -12.27) | 0.017 (0.016, 0.018) | 1.18 (1.05, 1.31) | 0.303 | 0.978     | -108.8 | -106.1 |

h0.5, respectively with 95% confidence interval. Additionally, in this work  $T_o$  and  $b_1$  were calculated ranging from -12.19 to -10.93°C and from 0.018 to 0.021°C-1.h0.5, respectively when the traditionally used direct modelling approach was employed. All these results showed that dynamic inverse modelling approach based on the Bayesian optimization algorithm could estimate the minimum temperature for the growth of *Pseudomonas spp.* counts in fish.

Another parameter, b2 directly relating to the lag phase duration of microorganism, was calculated as  $1.78 \pm 0.14$  (mean  $\pm 95\%$  confidence interval) for the Bayesian optimization algorithm in dynamic inverse modelling approach. These results are within the range of findings reported by KOUTSOUMANIS,<sup>13</sup> who calculated b2 with average value of 1.62 to 2.25, suggesting that the inverse dynamic modelling approach based on the Bayesian optimization algorithm can predict b2 parameter of *Pseudomonas spp.* counts in fish.

 $\mu_{_{max}}$  and  $\lambda$  are the most important critical parameters to describe the growth behaviour of microorganisms in food, and temperature is a key determinant for both growth parameters.<sup>9,19</sup> The kinetic parameters including  $\mu_{max}$  and  $\lambda$ belonging to Pseudomonas spp. counts in fish for each modelling approach are presented in Fig. 4. As it is expected, the figures demonstrate that  $\mu_{_{max}}$  increased and  $\lambda$  decreased because of rising storage temperature. Additionally,  $\mu_{max}$ and  $\lambda$  values of *Pseudomonas spp.* counts in fish obtained from the inverse dynamic modelling approach on the Bayesian optimization algorithm are within the range of findings obtained from twostep direct modelling approach considering 95% confidence interval. These results indicated that the inverse dynamic modelling approach on the Bayesian optimization algorithm can be used for predicting  $\mu_{max}$  and  $\lambda$  parameters of Pseudomonas spp. counts in fish and is an alternative way to traditionally used two-step modelling approach for estimating growth parameters of microorganisms.

The validation of the models is the fundamental process by which the prediction ability of developed models can be tested using previously published or new generated data. In this regard, internally collected  $\mu_{max}$  and  $\lambda$  parameters of *Pseudomonas spp.* in fish,<sup>13</sup> were used for assessing the prediction power of the



**Fig. 4.** The effect of storage temperature on a) the maximum growth rate and b) the lag phase duration calculated with different modelling approach.

| Storage<br>temp.(°C) | Observed kinetic parameters <sup>a</sup> |                             | Predicted kinetic parameters          |                             |  |                             |
|----------------------|--|-----------------------------|---------------------------------------|-----------------------------|--|-----------------------------|
| p ( -)               |  |                             | Direct one-step<br>modelling approach |                             | Inverse dynamic<br>modelling approach <sup>b</sup> |                             |
|                      | Maximum<br>growth rate<br>(log CFU/h)    | Lag time<br>duration<br>(h) | Maximum<br>growth rate<br>(log CFU/h) | Lag time<br>duration<br>(h) | Maximum<br>growth rate<br>(log CFU/h)              | Lag time<br>duration<br>(h) |
| 0                    | 0.054 ± 0.002                            | 37.2 ± 5.9                  | 0.042                                 | 33.7                        | 0.051  | 34.9                        |
| 2                    | 0.064                                    | 30.8                        | 0.064                                 | 22.2                        | 0.069  | 25.9                        |
| 3                    | 0.070                                    | 30.3                        | 0.076                                 | 18.5                        | 0.079  | 22.7                        |
| 5                    | 0.103 ± 0.007                            | 19.9 ± 2.8                  | 0.105                                 | 13.4                        | 0.100  | 17.8                        |
| 7                    | 0.130                                    | 12.5                        | 0.138                                 | 10.2                        | 0.124  | 14.3                        |
| 8                    | 0.137 ± 0.008                            | 13.0 ± 2.5                  | 0.156                                 | 9.0                         | 0.138  | 12.9                        |
| 10                   | 0.191 ± 0.009                            | 11.8 ± 1.2                  | 0.196                                 | 7.2                         | 0.166  | 10.7                        |
| 15                   | 0.269 ± 0.026                            | 8.1 ± 0.6                   | 0.316                                 | 4.5                         | 0.248  | 7.2                         |
|                      | $B_{f}$                                  |                             | 0.97                                  | 1.45                        | 1.02   | 1.09                        |
|                      | $A_{f}^{'}$                              |                             | 1.10                                  | 1.45                        | 1.07   | 1.13                        |

Table 2. Observed and predicted kinetic parameters of Pseudomonas spp. in fish stored at various temperatures

<sup>a</sup>Observed kinetic parameters of Pseudomonas spp. in fish were collected from the work of Koutsoumanis, (2001).

<sup>b</sup>Predicted kinetic parameters of *Pseudomonas spp.* in fish were obtained by Bayesian optimization algorithm.

 $B_{f}$  – Bias factor and  $A_{f}$  – Accuracy factor were calculated based on bacterial count of log CFU/g.

direct one-step modelling approach, which gave better goodness of fitting results between direct modelling approaches and the Bayesian optimization algorithm in inverse dynamic modelling approach considering  $B_f$  and  $A_f$  (Table 2). The statistical indices of Bf were 0.97 and 1.45 for the  $\mu_{max}$  and  $\lambda$  parameters using the direct one-step modelling approach, respectively. A  $B_f$  factor of 1 indicates no structural deviation of the model. The Bf factor of 0.97 for  $\mu_{max}$  parameter indicated that the one-step modelling approach underestimated 3% whereas the Bf factor of 1.45 for  $\lambda$  parameter indicated that the one-step modelling approach overestimated 45% when the direct one-step

modelling approach was employed. Additionally, the direct one-step modelling approach provided statistical indices of  $A_{f}$  1.10 and 1.45 for the  $\mu_{max}$ and  $\lambda$  parameters, respectively, meaning that on average the predicted values were 10% and 45% different from the observed values for the  $\mu_{max}$ and  $\lambda$  parameters, respectively. On the other hand, the inverse dynamic modelling approach based on the Bayesian optimization algorithm yielded suitably statistical indexes  $(1.02 > B_f >$ 1.09 and 1.07 >  $A_f$  > 1.13) confirming that the inverse dynamic modelling approach based on the Bayesian optimization algorithm considerably improved models' prediction capability of  $\mu_{\scriptscriptstyle max}$ and  $\boldsymbol{\lambda}$  parameters and can be reliably used as an alternative way of describing the growth behaviour of Pseudomonas spp. in fish

## CONCLUSION

In this work, the Baranyi model was used for evaluating fitting capabilities of direct twostep, one-step and inverse dynamic modelling approaches. The direct one-step modelling approach improved the fitting capability of the Baranyi model used in two-step direct modelling approaches. The inverse dynamic modelling approach based on each of the used optimization algorithms provided better goodness of fit results compared to direct modelling approaches (twostep and one-step modelling approaches), but the Bayesian optimization algorithm was the best. The inverse dynamic modelling approach based on the Bayesian optimization algorithm provided similar results for the parameters of  $\mu_{max}$ and  $\lambda$  of *Pseudomonas spp.* in fish to two-step direct and one-step direct modelling approaches, meaning that the inverse dynamic modelling approach based on the Bayesian optimization algorithm has a considerable potential to be used as an alternative simulation method to the direct two-step modelling approach, most commonly used in predictive microbiology, by which the microbiological quality of the food products can be accurately and fast monitored.

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#### **CONFLICT OF INTEREST**

The authors declare that there is no conflict of interest.

## **AUTHORS' CONTRIBUTION**

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

#### FUNDING

None.

## DATA AVAILABILITY

All datasets generated or analyzed during this study are included in the manuscript.

## **ETHICS STATEMENT**

Not applicable.

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