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Bioinactivation FE: A free web application for modelling isothermal and dynamic microbial inactivation

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ABSTRACT

Mathematical models developed in predictive microbiology are nowadays an essential tool for food scientists and researchers. However, advanced knowledge of scientific programming and mathematical modelling are often required in order to use them, especially in cases of modelling of dynamic and/or non-linear processes. This may be an obstacle for food scientists without such skills. Scientific software can help making these tools more accessible for scientists lacking a deep mathematical or computing background.

Recently, the R package *bioinactivation* was published, including functions (model fitting and predictions) for modelling microbial inactivation under isothermal or dynamic conditions. It was uploaded to the Comprehensive R Archive Network (CRAN), but users need basic R programming knowledge in order to use it. Therefore, it was accompanied by *Bioinactivation SE*, a user-friendly web application including selected functions in the software for users without a programming background.

In this work, a new web application, *Bioinactivation FE,* is presented. It is an extension of *Bioinactivation SE* which includes an interface to every function in the *bioinactivation* package: model fitting of isothermal and non-isothermal experiments, and generation of survivor curves and prediction intervals. Moreover, it includes several improvements in the user interface based on the users' feedback. The capabilities of the software are demonstrated through two case studies using data published in the scientific literature. In the first case study, the response of *Escherichia coli* to isothermal and non-isothermal treatments is compared, illustrating the presence of an induced thermal resistance. In the second, the effect of nanoemulsified D-limonene on the thermal resistance of *Salmonella* Senftenberg is quantified.

1. Introduction

Several efforts have been dedicated to developing approaches for ensuring the safety and quality of food products. Various methods have been applied, advancing from qualitative towards quantitative approaches and risk assessments (Coleman & Marks, 1999; Lindqvist, Sylvén, & Vågsholm, 2002). These methods require an accurate description of microbial responses in the whole food chain, i.e. during harvesting, processing, distribution, storage, preparation and consumption. In this respect, predictive microbiology has proved its applicability to achieve this purpose.

Predictive microbiology is based on the hypothesis that past experience can be used to predict the microbial response (Ross, 1996). Therefore, data generated under laboratory conditions can be used to estimate the microbial concentration during the farm-to-fork life of the product using mathematical models (McMeekin, Olley, Ratkowsky, & Ross, 2002). The first scientific papers on predictive microbiology date from the early 1920s, when the inactivation kinetics of *Clostridium botulinum* spores during isothermal treatments was studied (Bigelow, 1921; Bigelow & Esty, 1920; Esty & Meyer, 1922). However, its applicability was quite limited until the 1980s, most likely due to the limited computational power available at the time. Nowadays, predictive microbiology models are basic tools for food safety studies and quantitative risk assessment (McMeekin, Mellefont, & Ross, 2007).

However, the application of mathematical models is still, to some extent, limited. This is likely due to the absence of stand-alone software solutions, and the lack of free open databases and software (Plaza-Rodríguez et al., 2015). Furthermore, many food microbiologist lack

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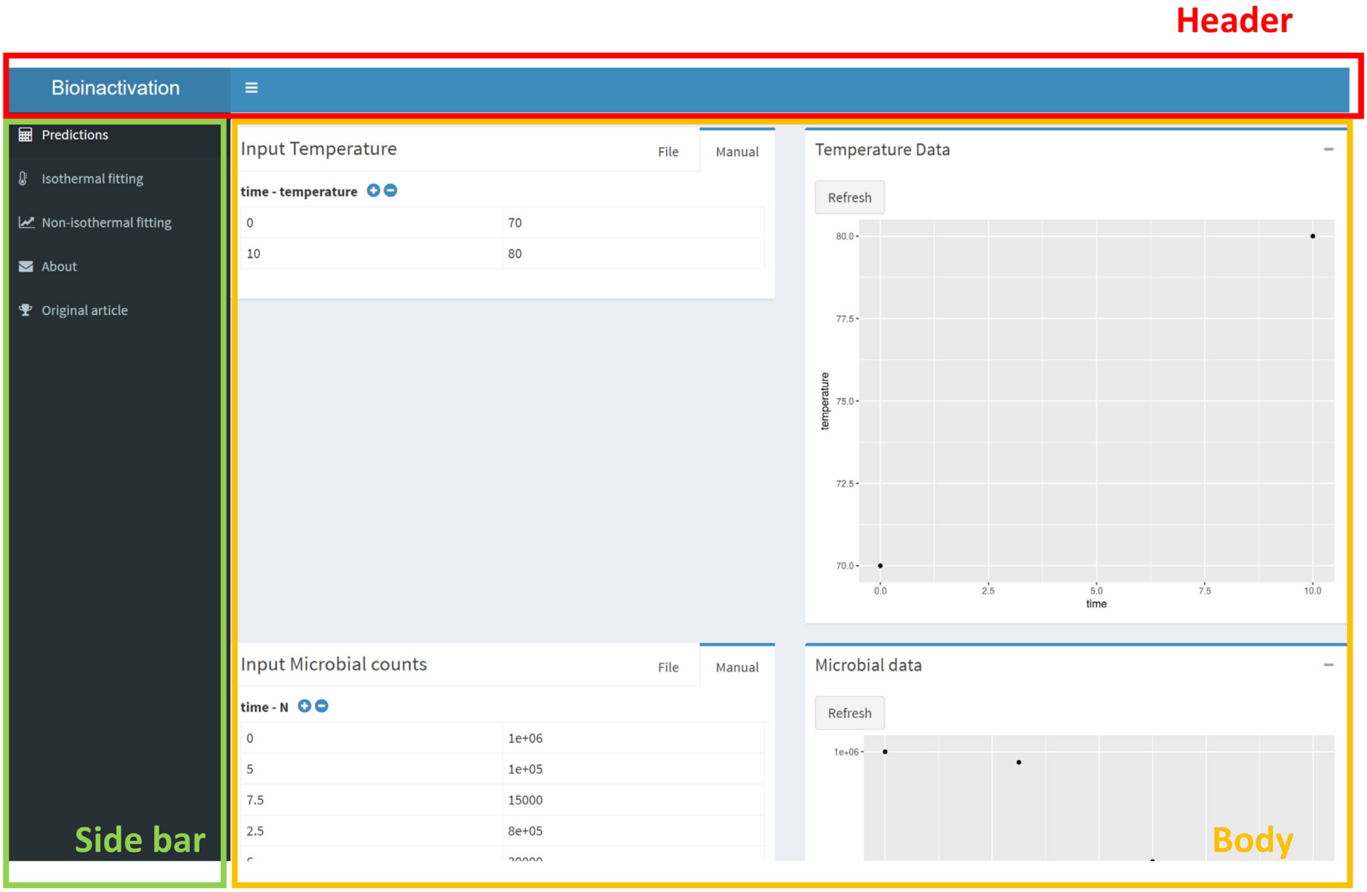

time - temperature

0	70
10	80

time - N

0	1e+06
5	1e+05
7.5	15000
2.5	8e+05

Fig. 1. Overview of the layout of *Bioinactivation FE* as it is loaded by the web browser.

the necessary skills in statistics, mathematical modelling and scientific programming required to develop and apply mathematical models (Granato, de Araújo Calado, & Jarvis, 2014; Granato, Nunes, & Barba, 2017; Nunes, Alvarenga, Santos, and Granato, 2015). A way to circumvent these limitations is the development of user-friendly software applications, so that mathematical models can be used and their results interpreted by users without advanced education in mathematical modelling and software development (Muñoz-Cuevas, Metris, & Baranyi, 2012).

A recent review article described the software tools presented at the International Congress of Predictive Microbiology in Foods in 2013 (ICPMF8) software fair (Tenenhaus-Aziza & Ellouze, 2015). However, none of the freely available software included all the tools required to model microbial inactivation: fitting of isothermal and non-isothermal experiments, and generation of predictions under dynamic and static conditions (Garre, Fernández, Lindqvist, & Egea, 2017). Since the review by Tenenhaus-Aziza & Ellouze, two new free applications have been developed: IPMP Global Fit and bioinactivation. IPMP Global Fit (Huang, 2017) is a tool for curve fitting of isothermal growth and inactivation experiments but it does not generate predictions. It is freely available and its files are downloaded and executed locally. Bioinactivation (Garre et al., 2017) includes functions for the model fitting of both isothermal and non-isothermal experiments, as well as for generating predictions. It is available as an R package (*bioinactivation*), and uploaded to CRAN making it publicly available as an open software (https://CRAN.R-project.org/package=bioinactivation). The use of the *bioinactivation* package requires basic knowledge of R programming from the user. For that reason, a user-friendly web interface including only the functions for model fitting of iso- and non-isothermal experiments was developed: *bioinactivation SE* (https://opada-upct.shinyapps.io/bioinactivation_SE/).

Thus, the R package *bioinactivation* includes all the functions usually required for mathematical modelling of microbial inactivation (model fitting and generation of predictions for isothermal and dynamic conditions), but there is no free user-friendly application including all these functions. Consequently, due to the positive feedback received from the users of *bioinactivation*, a novel web application, *Bioinactivation FE*, described in the present work has been developed. This application includes an interface to all functions in the *bioinactivation* package. In this article, the capabilities of *Bioinactivation FE* are showcased through two different case studies using data already published in the scientific literature. The first compares the inactivation patterns of *Escherichia coli* during isothermal and non-isothermal treatments, whereas the second assesses how different concentrations of nanoemulsified D-limonene affects the thermal inactivation of *Salmonella* Senftenberg. Besides, a general description of the functions implemented and the user interface is provided.

2. Materials and methods

2.1. Bioinactivation FE

Bioinactivation FE is a user-friendly interface to all the functions included in the *bioinactivation* package for R (Garre et al., 2017); i.e. simulation of survivor curves, generation of prediction intervals, and model fitting of isothermal and dynamic experiments. It has been built using the *shiny* (Chang, Cheng, Allaire, Xie, & McPherson, 2017) and *shinydashboard* (Chang & Ribeiro, 2017) packages. The combination of both packages allows the creation of a web page with input and output widgets able to run R code in the background (R Core Team, 2016). Therefore, users can access advanced mathematical operations implemented in R without any skills in this programming language.