



IPMP 2013 – A comprehensive data analysis tool for predictive microbiology[☆]



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ABSTRACT

Predictive microbiology is an area of applied research in food science that uses mathematical models to predict the changes in the population of pathogenic or spoilage microorganisms in foods exposed to complex environmental changes during processing, transportation, distribution, and storage. It finds applications in shelf-life prediction and risk assessments of foods. The objective of this research was to describe the performance of a new user-friendly comprehensive data analysis tool, the Integrated Pathogen Modeling Model (IPMP 2013), recently developed by the USDA Agricultural Research Service. This tool allows users, without detailed programming knowledge, to analyze experimental kinetic data and fit the data to known mathematical models commonly used in predictive microbiology. Data curves previously published in literature were used to test the models in IPMP 2013. The accuracies of the data analysis and models derived from IPMP 2013 were compared in parallel to commercial or open-source statistical packages, such as SAS® or R. Several models were analyzed and compared, including a three-parameter logistic model for growth curves without lag phases, reduced Huang and Baranyi models for growth curves without stationary phases, growth models for complete growth curves (Huang, Baranyi, and re-parameterized Gompertz models), survival models (linear, re-parameterized Gompertz, and Weibull models), and secondary models (Ratkowsky square-root, Huang square-root, Cardinal, and Arrhenius-type models). The comparative analysis suggests that the results from IPMP 2013 were equivalent to those obtained from SAS® or R. This work suggested that the IPMP 2013 could be used as a free alternative to SAS®, R, or other more sophisticated statistical packages for model development in predictive microbiology.

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1. Introduction

Predictive microbiology is an area of research in applied food science that applies mathematical models to describe the dynamics (growth and survival) of the populations of microorganisms undergoing complex physical, chemical, and biological changes in the environment during processing, transportation, distribution, and storage of foods. Emerging as an active area of research in the 1980s (Buchanan, 1993; McMeekin et al., 1993), predictive microbiology has become a useful tool in microbial shelf life prediction, quality control, and risk assessments.

According to Whiting and Buchanan (1993), mathematical models used in predictive microbiology could be generally categorized into three types, including the primary, secondary, and tertiary models. The primary models are the mathematical models that describe the

change in the microbial population as a function of time under a single set of conditions (Baranyi and Roberts, 1995; Buchanan et al., 1997; Gibson et al., 1987; Huang, 2008, 2013; Zwietering et al., 1990). The secondary models are the mathematical models that describe the responses of one or more parameters of a primary model to one or more environmental conditions (Buchanan et al., 1989; Huang et al., 2011a, 2011b; Ratkowsky et al., 1983; Rosso et al., 1993). The tertiary models are computer software or expert systems that utilize the primary and secondary models to predict the fate of microorganisms in foods. The primary and secondary models are the foundation for building a tertiary model.

Since the 1980s, significant progress has been achieved in predictive microbiology research and application. The development and availability of the USDA Pathogen Modeling Program (PMP), its companion product, USDA Pathogen Modeling Program Information Portal (PMIP), and ComBase, represents desktop and online applications of tertiary models. For data analysis and model curve-fitting, DMFit (primarily for Baranyi model, available from <http://www.ifr.ac.uk/safety/dmfit/>) and GinaFit (for microbial survival models, available from <http://cit.kuleuven.be/biotec/downloads.php>) are two well-known Excel add-in packages for primary model development. There is a

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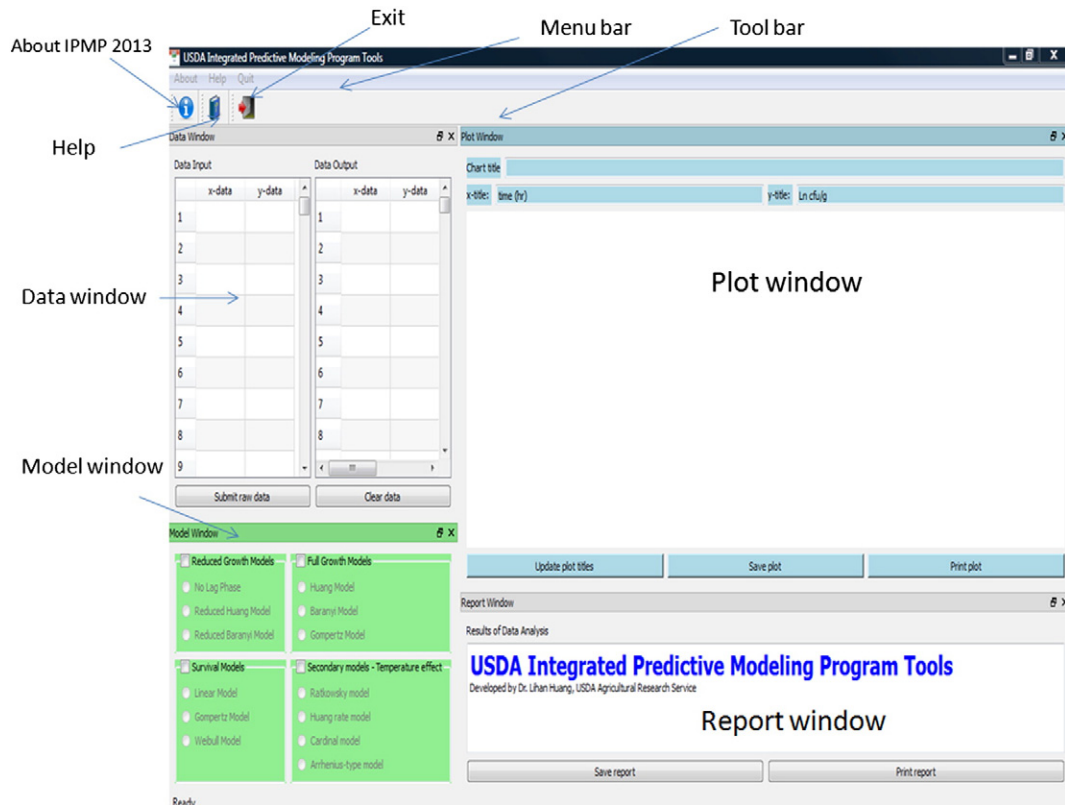


Fig. 1. Graphical user interface (GUI) for IPMP 2013.

need, however, for a comprehensive data analysis tool for both primary and secondary models. Many researchers also use commercially available general-purpose statistical analysis and mathematical tools, such as SAS®, MATLAB®, Mathematica®, S-Plus®, or SPSS®, while others use open-source statistical analysis tools, such as R, for data analysis. These general-purpose tools, unfortunately, require product-specific programming. For someone lacking programming knowledge, it can be difficult to use these tools effectively. In addition, commercial statistical packages and math tools are expensive and usually require annual maintenance or license fees.

Therefore, the objective of this research was to develop a comprehensive data analysis tool, i.e., the USDA Integrated Pathogen Modeling Program (IPMP 2013), for both primary and secondary models. The specific aim of this work was to develop an easy-to-use data analysis platform, equipped with user-friendly graphical user interfaces (GUI), for developing predictive models. The ultimate goal was to develop a data analysis tool that would allow anyone, with a basic knowledge of predictive microbiology, to use it to analyze kinetic data and develop predictive models for microorganisms in foods without the need of computer programming.

2. Materials and methods

2.1. Software design and components

IPMP 2013 was developed using open-source technologies, and is available online for download and evaluation (<http://www.ars.usda.gov/Main/docs.htm?docid=23355>). The software was written in Python (www.python.org), a modern object-oriented scripting language that can be operated under various operating systems, including Microsoft Windows, Mac OS X, and Linux/Unix. The graphical user interfaces were developed using PyQt4, Python binding of the Qt (v4) cross-

platform application framework (qt-project.org). PyQt4 was developed by Riverbank Computing Limited (UK). The software is periodically upgraded to expand its capacities and enhance its performance. Fig. 1 illustrates the structure of user interfaces for IPMP 2013.

The software was designed with 4 GUI components or sub-windows, including the Data Window, Model Window, Plot Window, and Report Window (Fig. 1). The Model, Plot, and Report Windows were custom-designed for IPMP 2013. The Data Window was adopted from an open-source Python code originally developed for Opensesame, which is an open-source experiment builder for the social sciences (<http://osdoc.cogsci.nl/index.html>). The Plot Window was based on another open-source product – matplotlib (Hunter, 2007), available from www.matplotlib.org.

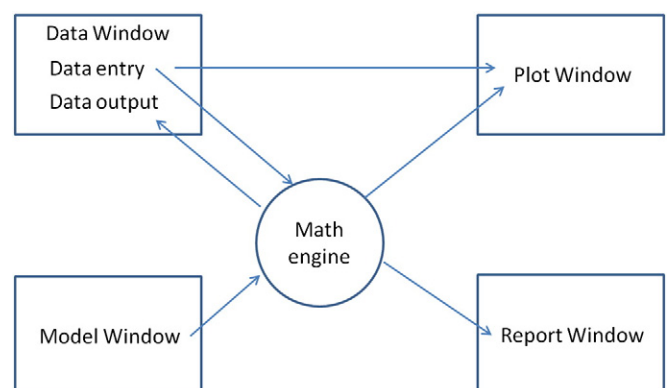


Fig. 2. The flow of data in IPMP 2013.

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