PREDICTIVE MODELLING UNDER DYNAMIC CONDITIONS IN FOOD PROCESSING ENVIRONMENTS

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ABSTRACT

Commercial thermal and non-thermal processes for food are dynamic, where temperature, water activity, and other variables can change with time. An efficient process design requires knowing the parameters of microbial mathematical models describing the underlying dynamic processes. However, most research to obtain these parameters is performed under simulated constant conditions. The objective of this session is to address some of the recent developments to model predictive microbial dynamics of food processes describing examples on how to perform inverse (parameter estimation) problems for a number of different primary-secondary models. Therefore, appropriate experimental designs, such as optimal experimental design, parameter identification under dynamic conditions, and properly statistical indices to discriminate among models are discussed.

DYNAMIC ENVIRONMENTS

The majority of most food technologies are dynamic in nature. The main changing processing factor is temperature and its impact to biological/chemical reponses in most cases is significant and can result in induced microbial/chemical stress responses hence making some processes less effective. Some examples, include the classical pasteurization and sterilation treatments which include nonisothermal heating-up phases and temperature fluctuations during the process. Others include adiabatic heating during the application of High Hydrostatic Temperautre (e.g., Valdramidis et al., 2009) and high-pressure carbon dioxide processing (Garcia-Gonzalez et al., 2009) as well as the increase of the temperature during the application of Pulsed Electric Field (PEF) processing inside PEF chambers (Jaeger et al. , 2010). Nevertheless, the chemical, microbial, and enzymatic responses as they change during these processing conditions are usually studied assuming that operations are applied at static conditions.
In this approach, the kinetic parameters of a model describing the evolution of the concentration of a component (e.g., chemical, microbial) over time are estimated for at least three different static environmental conditions. These estimates are correlated with the tested conditions in order to identify the kinetic parameters of interest. Hereafter, a validation step is applied usually under dynamic conditions. If predicted and measured results are close to each other, this closeness can confirm the assumption that parameters derived from static conditions are nearly equal to parameters during dynamic conditions.
Despite the easiness of the implementation of this modeling methodology, also known as two-step modeling methodology, its drawabcks will be discussed in this session and it will be highlighted that even if the results are excellent following the use of isothermal inactivation parameters, one does not know the actual values of nonisothermal estimates. Concluding, the importance to apply parameter identification techniques under dynamic conditions representative of a realistic (processing) environment will be introduced.

OPTIMAL EXPERIMENTAL DESGIN

Both the selection of an appropriate model structure and the identification of accurate model parameters are data-driven processes. Therefore, the quality of the experimental data is critical for appreciating the efficiency and accuracy of these procedures. Experimental data should be informative enough and this could improve the model building and parameter estimation. A novel methodology for the collection of more informative data via dynamic input profiles (e.g., temperature) is based on the concepts of Optimal Experiment Design for Parameter Estimation (OED/PE). In OED the (time-varying) process inputs are designed such that the resulting process outputs have maximum information content, and this within the validity region of the proposed process operation.

This methodology has been applied on traditional thermal processes (sterilization or mild heating) for microbial and chemical inactivation kinetics (Balsa-Canto et al., 2007; Cunha et al., 1997; Versyck et al., 1999) as well as on microbial growth studies (e.g., Van Derlinden et al., 2008, 2010, 2013).

Most applications of OED in food science focus on D-optimal design, which aims at maximizing the determinant of an information matrix. It has been proven that optimal experimental design can significantly reduce the number of experiments and increase the accuracy of parameters by indicating the best times to collect data. Presuming model validity, the mathematical technique of optimal experiment design for parameter estimation (OED/ PE) can be designed to estimate accurate and precise parameters. When applying dynamic experiments, this approach also guarantees parameter estimates which are valid under varying, more realistic conditions

Thereofore, this session will also focus on the importance of experimental data collection for the modelling of bioprocesses. The various steps towards accurate bioprocess models will be revised. The concepts of OED will be outlined while optimal dynamic experiment design for parameter estimation of the Ratkowsky square root model will be presented as case study. In addition, novel developments as the integration of multiple objectives will be discussed. In particular criteria which aim at a better conditioning of the system, i.e., the modified E-criterion or anti-correlation criteria, and criteria which aim at the global maximization of the information content will be discussed. Furthermore, a more recent trend of integrating the final goal of the model in the optimal experiment design procedure will be highlighted (Houska et al., 2015).

INVERSE PROBLEM IN REALISTIC ENVIRONMENTS

Previous studies have shown that non-isothermal microbial inactivation parameters can be estimated accurately and precisely with a minimum of experiments collected under realistic processing conditions, even without the application of OED, and by applying either ordinary least squares nonlinear regression or a sequential procedure. This session will also focus on presenting tools that can be applied to rate-dependent parameters in food safety computations. Methods such as OLS and sequential estimation will be demonstrated and presented as alternatives to numerous isothermal experiments and multiple-step linear regression, which typically have too few degrees of freedom to attain desirable small standard error for microbial models.

The main key points of this session will be to demonstrate that non-static microbial kinetic model parameters could be accurately and precisely estimated using one-step nonlinear regression following an ordinary least squares and a sequential approach (Dolan et al., 2013); and to demonstrate the use of appropriate statistical indices on choosing the best performing out of different differential models (Dolan and Mishra, 2013).

Even after the parameters have been accurately estimated there will remain a level of uncertainty. In order to deliver accurate predictions the uncertainty on the model predictions have to be accounted for. The accurate propagation of uncertainty of a stochastic nature can be performed by employing smart sampling based techniques as the unscented transformation (Julier96).

CONCLUSIONS

This tutorial will focus on the advances in predictive microbial dynamics of food processes for estimating accurate and precise modeling parameters that can reliably be used to predict realistic processing conditions. The need a a problem statement for dynamic modeling approaches will be showcased and appropriate experimental designs, such as optimal experimental design, parameter identification under dynamic conditions, and properly statistical indices to discriminate among models will be discussed.

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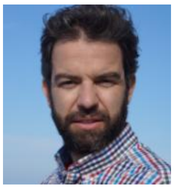
AUTHOR BIOGRAPHIES



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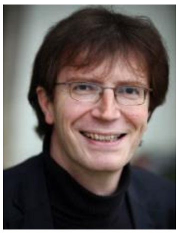

JAN VAN IMPE is a full professor at the chemical engineering department of KU Leuven. He obtained his MSc from the University of Gent in 1988, and his PhD from the KU Leuven in 1993. Immediately thereafter he founded the BioTeC (Chemical and Biochemical Process Technology and Control) research group [www.cit.kuleuven.be/biotec]. In the period 2005-2011 he has served as Departmental Head. He has been visiting professor at the UA (University Antwerpen) [2006-2015]. He is a founding partner of the KU Leuven Center-of-Excellence OPTEC (Optimization in Engineering) in 2005, and at present he is coordinating OPTEC's continuation (Phase II: 2010-2017 www.kuleuven.be/optec). In 2008 he started the Flemish Cluster for Predictive Modeling in Foods [www.cpmf2.be], to facilitate the transfer of the broad expertise in the area of predictive microbiology to industry/government. From 2009-2014 on, he held the essenscia-chair, funded by the Belgian Chemical and Life Sciences Industry platform [www.scores4chem.be].